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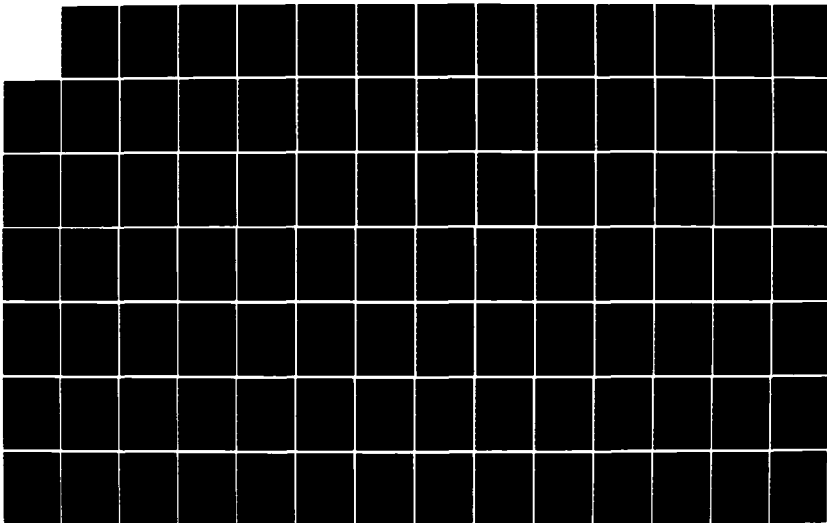
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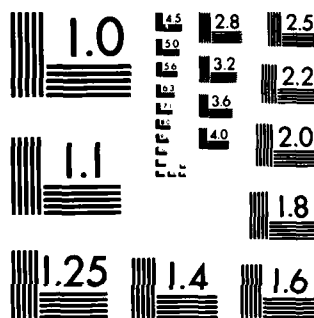
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AN INTERACTIVE COMPUTER PACKAGE FOR USE  
WITH SIMULATION MODELS WHICH PERFORMS  
MULTIDIMENSIONAL SENSITIVITY ANALYSIS  
BY EMPLOYING THE TECHNIQUES OF  
RESPONSE SURFACE METHODOLOGY

THESIS

Presented to the Faculty of the School of Engineering  
of the Air Force Institute of Technology  
Air University  
In Partial Fulfillment of the  
Requirements for the Degree of  
Master of Science in Operations Research

Kalla J. Sparrow, B.A.  
First Lieutenant, USAF

December 1984



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Abstract

↙ The overall objective of this research effort was to develop an interactive, user-friendly response surface methodology computer package which can be attached to any FORTRAN based simulation model to yield a response function which describes the relationships between the input parameters and the output parameter of interest. Subobjectives were:

- (1) After the response surface is generated, search this surface for the combinations of pertinent input parameters that yield the optimum response,
- (2) Interpret how the response function reveals the sensitivity of the output parameter due to changes in input parameters, and
- (3) Illustrate how the response function describes the relative ranking of effects on response between input parameters.

This research effort accomplished the overall objective and touched on subobjectives two and three.

The overall objective was accomplished by developing the RSM computer program. The user-friendly requirement meant the program had to be flexible and easy to understand. The input requirements were designed to be easily understood and proceed in a logical sequence. Five design types are offered by this program and also a user design input subroutine offers further flexibility. The first-order design types offered are the full  $2^k$  and the fractional  $2^{k-P}$  designs and the second-order design types offered are the full  $3^k$ , the fractional  $3^{k-P}$ , and the central composite designs, where  $k$  is the number of factors. This RSM program can handle from two to nine factors. This RSM program can handle from two to nine factors. The user can use the regression portion offered by this program or can choose to use the permanent file 'MATRIX', which is generated containing necessary data, to perform his/her own statistical analysis. The RSM program's modular design enables enhancements to be made with few changes to the program itself.

Subobjectives two and three were implicitly accomplished by the output displayed from the regression portion. The estimated coefficients and associated statistics illuminate the relationships between the input factors and reveal sensitivities in the response due to changes in input factors.

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## Preface

This research effort could not have been accomplished without the help of many others. I am indebted to my co-advisors, Lt. Col. Ivy Cook and Lt. Col. Palmer Smith, for their continued suggestions and encouragements. Without their guidance, the objectives of this research would never have been realized. I also wish to thank Maj. James Coakley for his assistance in supplying a simulation model and for his many hours of help during the program application phase of this research effort. Finally, I wish to thank my family. I thank my sons, Donald and Jeff, for their tolerance and hope that someday they will understand why there were many days and nights I could not be with them. Most of all, I thank my husband Don for his awareness of my feelings during this trying period and the many nights he sacrificed sleep to type this thesis to insure my completion of this program.

**Kalla J. Sparrow**

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Abstract

The overall objective of this research effort was to develop an interactive, user-friendly response surface methodology computer package which can be attached to any FORTRAN based simulation model to yield a response function which describes the relationships between the input parameters and the output parameter of interest.

Subobjectives were:

(1) After the response surface is generated, search this surface for the combinations of pertinent input parameters that yield the optimum response,

(2) Interpret how the response function reveals the sensitivity of the output parameter due to changes in input parameters, and

(3) Illustrate how the response function describes the relative ranking of effects on response between input parameters.

This research effort accomplished the overall objective and touched on subobjectives two and three.

The overall objective was accomplished by developing the RSM computer program. The user-friendly requirement meant the program had to be flexible and easy to understand. The

input requirements were designed to be easily understood and proceed in a logical sequence. Five design types are offered by this program and also a user design input subroutine offers further flexibility. The first-order design types offered are the full  $2^k$  and the fractional  $2^{k-p}$  designs and the second-order design types offered are the full  $3^k$ , the fractional  $3^{k-p}$ , and the central composite designs, where  $k$  is the number of factors. This RSM program can handle from two to nine factors. The user can use the regression portion offered by this program or can choose to use the permanent file 'MATRIX', which is generated containing necessary data, to perform his/her own statistical analysis. The RSM program's modular design enables enhancements to be made with few changes to the program itself.

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I. Introduction

Background

A complex system typically cannot be studied by analytical methods. Moreover, in order to gain insight into how the system operates, analysts must model all aspects of the system structure. Thus, in the current environment, many problems of operations research and management science must be attacked by means of computer simulation.

A computer simulation can be thought of as a black box where input parameters or factors enter the complex system and through some process act and are acted upon to produce an (several) output(s). For example, in a hospital emergency room, input variables might be the arrival rate of patients, the severity of the emergency, and the number of doctors, nurses, and technicians on duty. An output parameter might be the time a patient waits for service. Another example is a model which analyzes conventional weapons effectiveness. Input variables could be the number of attacks allowed, the number of targets, and the number of weapon patterns, and possible outputs might be the probability of denying aircraft operations and expected values for number of hits and area damaged. Still another example is a model of Army cargo

aircraft scheduling. The model's objective is to maximize an overall score which represents the satisfaction of the end user. The Army distinguishes nine types of supply classes. The priorities given to these supply classes are the model's inputs and affects the end user's satisfaction level.

There are two types of input parameters -- controllable factors and uncontrollable factors. Controllable factors are those input parameters having values which may be directly controlled by the decision maker in the real world, and uncontrollable factors are those over which the decision maker has no direct control. From the previous hospital emergency room example, the arrival rate of patients and the severity of the emergency are uncontrollable factors, and the controllable factors would be the number of doctors, nurses and technicians assigned on duty.

Typically these complex systems are studied with some purpose in mind. In the case of the hospital emergency room, personnel may be interested in monitoring patient flow and determining those values of controllable input parameters which minimize patient waiting time. Similarly, in the model of a conventional weapons exercise, analysts want to determine those combinations of controllable input parameters which produce the maximum weapon effectiveness (a measurable quantity). Which input factors have relatively little impact on the output parameter of interest? Which input factors have the most impact on the output parameter of interest? For any simulation model, it is desirable to explicitly

express the relationships between the input factors and output factors which are implicitly defined within the computer code of the simulation model.

#### Problem Statement

There are two methods available to aid in determining these relationships -- internal methods or external methods. The internal method is accomplished by the programmer changing the structure of the system until an acceptable result is achieved. In large simulation models this method is not feasible. The internal method requires unreasonable amounts of time and is not easy to implement. Recently analysts have been customizing the external technique of response surface methodology to gain insight into how an output parameter responds to changes in combinations of input factors. There are several advantages to this external method. Once generated, the response surface reveals the relative importance of the input factors to the output and also illuminates the interdependence between pertinent factors within the system. Furthermore, once generated the response surface can be searched to determine that combination of factor inputs which produces the optimum response. The drawback with customizing response surface methodology to a simulation model is that in order to implement this type of technique, an analyst must understand the mathematics and statistical theory involved. What is needed is an external method that employs response surface

methodology which an analyst can use in combination with a simulation model without needing to understand all the mathematics and statistical theory involved.

#### Research Question

Can a general response surface computer package be developed which can be attached to any FORTRAN-based simulation model to yield as output the description of the response surface dependent upon the controllable input parameters?

#### Research Objectives

The overall objective of this research is to develop an interactive, user-friendly response surface computer package which can be attached to any FORTRAN-based simulation model to yield a response function which describes the relationships between the input parameters and the output parameter of interest. To insure that any computer package is used to its potential, it must meet user needs. Because of this desirable property, the response surface methodology computer package is developed with ease of user interface and minimum programming experience as primary considerations. Another requirement to meet user needs is that the computer package be portable between computer systems used by simulation models.

Subobjectives of this research effort are as follows:

- (1) After the response surface is generated, search this surface for the combinations of pertinent input

parameters that yield the optimum response,

(2) Interpret how the response function reveals the sensitivity of the output parameter due to changes in input parameters, and

(3) Illustrate how the response function describes the relative ranking of effects on response between input parameters.

### Scope

Limitations exist in any research effort. Some limitations of this research effort are:

(1) The controllable factors are continuous, or if discrete, for arithmetic purposes it is reasonable that they can be assumed to be continuous,

(2) There is a single output specified to be used in the analysis,

(3) The user will be allowed to vary only two to nine input parameters,

(4) The user must define input variables in terms of a high and low value, and

(5) Only first-order and second-order designs will be considered.

### Summary

This chapter briefly discussed the background, problem statement, research question, objectives, and scope pertaining to this research effort. The next chapter discusses the literature review conducted during this

research effort.

## II Literature Review

The actual programming of the response surface methodology computer package requires knowledge of: (1) Computer Simulation Experiments, (2) Statistical Experimental Design, (3) Response Surface Methodology, (4) Regression Analysis, and (5) Applications of Response Surface Methodology.

### Computer Simulation Experiments

Before discussing simulation experiment objectives and alternatives, it is important to clarify some basic terms.

In Hunter and Naylor's article "Experimental Designs for Computer Simulation Experiments", they define simulation as "... a numerical technique for conducting experiments with certain types of mathematical models describing the behavior of a complex system on a digital computer over extended periods of time." (28:423) Because simulation models are developed to copy real-world systems, they, themselves, become very complex.

Simulation models are characterized by: (1) many variables and their functions; (2) stochastic variables and their distributions; (3) many parameters; (4) many linkages between elements of the model; (5) nonlinearities; (6) assorted constraints; and (7) a response (or responses) that may or may not have a time path. (28:423)

This quote basically means that a simulation model has a response (or responses) which is dependent upon many different factors. Some of these factors are deterministic (their values remain constant) and some are stochastic (their

values depend on probability distributions). Each of the factors has a unique effect on the response and some factors (or all) may have a joint effect on the response. There may be certain constraints included in the model which restrict the response region or factors included in the model, and the response may vary as a function of time.

After the simulation model is developed and validated (the simulated data are within some error tolerances of actual and historic data of the real-world system), the analyst desires to answer certain questions about the model, thereby answering questions about the true system. To quote an article: "The experimenter should specify his objectives as precisely as possible to facilitate the choice of a design which will best satisfy his objectives." (32:1332) With a simulation model two main objectives can be identified: (1) the experimenter wishes to find the combination of factor levels at which the response variable is maximized (or minimized) in order to optimize some process, and (2) the experimenter wishes to make a rather general investigation of the relationship of the response to the factors in order to determine the underlying mechanisms governing the process under study. (32:1333)

The two most popular techniques used to analyze simulated data are regression analysis and analysis of variance. As mentioned previously, the objective might be to explore and describe, over a specified experimental region, the response surface, or the objective might be to optimize



the response over a realistic experimental region. In either case, to satisfy the objective(s) data must be collected. These data consist of observations of the response at various levels of each of the factors. The typical experimental designs used are: full factorial designs, fractional factorial designs, and response surface designs. (24:424)

### Experimental Designs

There are many types of experimental designs available today. The majority of these designs can be classified into one or more of the following groups: single-factor experiments like randomized block and latin square designs; factorial experiments ( $2^k$  and  $3^k$ ); nested and nested-factorial experiments; split-plot factorial designs; fractional factorial experiments with and without blocking; and, response surface designs. It is not necessary to discuss in detail each of these types of experimental designs, because excellent texts on experimental design are readily available, including: The Design and Analysis of Industrial Experiments published in 1963 (10); Cochran and Cox's classic Experimental Designs of which several editions are available (16); and, most recently, Fundamental Concepts in the Design of Experiments by Charles Hicks (25). If a listing of experimental design literature is needed, although published in 1969, Herzberg and Cox's "Recent Work on the Design of Experiments: A Bibliography and a Review" is a superb source. Their article

groups the designs within the bibliography by type so that articles and texts dealing with a particular area are easily located. (24)

The experimental designs pertinent to this research effort were: factorial designs, fractional factorial designs, and response surface designs. To reiterate, the purpose of using experimental designs in simulation is to minimize the number of observations needed, and/or minimize the error associated with the results obtained, and/or minimize the chance of describing the surface incorrectly. At the same time, the experimenter desires to obtain results which will satisfy his objectives.

Full factorial designs and fractional factorial designs, both of which are used in response surface methodology, can be used with both qualitative and quantitative factors. When an analysis of variance technique is used, qualitative factors are acceptable because the objective is to determine which factors have a significant effect on the response. However, when these designs are used to fit a response surface, the factors must be quantitative (and be continuous or have enough discrete levels so that the factor can for all practical purposes be assumed continuous).

For this research effort, since it is assumed the response surface can be approximated by a low order polynomial, designs were needed which permitted fitting a first-order or second-order response surface over the experimental region. For example, for two controllable

factors,  $X_1$  and  $X_2$ , and a response  $Y$ , the first-order model would be:  $Y = B_0 + B_1X_1 + B_2X_2 + e$ , where the  $e$ 's are assumed to be identical, independent normally distributed errors with mean zero and variance  $\sigma^2$ . Table I gives the equations for first-order and second-order models.

The designs used to estimate first-order models are the full  $2^k$  factorial designs and the fractional  $2^k$  factorial designs. The controllable factors used in the experiment are input at 2 levels -- their high level and their low level. The full  $2^k$  factorial design requires that at each combination of factor levels an observation of the response is taken. This means that for a full  $2^k$  factorial design, two raised to the number of factors observations are required. The information that can be obtained from this quantity of runs is all the main effects and all the possible interaction effects. For instance, in a three-factor full factorial experiment,  $2^3$  observations would be taken. Estimates could be obtained for the relative effects on response due to  $X_1$ ,  $X_2$ , and  $X_3$ . Also, estimates could be made of the relative effects on response due to the two-factor interactions --  $X_1X_2$ ,  $X_1X_3$ , and  $X_2X_3$ . Furthermore, an estimate could be made of the relative effect on response due to the three-factor interaction --  $X_1X_2X_3$ . The problem is that it is difficult to interpret the meaning of high-order interactions. An extreme example would be with five factors. The number of observations required to run the full factorial experiment would be 32. There would be 5 main

TABLE I  
Two-Variable Designs

First-order assumed model implicit in simulation code	$Y = B_0 + B_1 X_1 + B_2 X_2$
Second-order assumed model implicit in simulation code	$Y = B_0 + B_1 X_1 + B_2 X_2 + B_{11} X_1^2 + B_{22} X_2^2 + B_{12} X_1 X_2$
Estimated Response Surface of Y First-order design	$\hat{Y} = b_0 + b_1 X_1 + b_2 X_2$
Estimated Response Surface of Y Second-order Design	$\hat{Y} = b_0 + b_1 X_1 + b_2 X_2 + b_{11} X_1^2 + b_{22} X_2^2 + b_{12} X_1 X_2$

Key

Y - the assumed true responses of the simulation model

$X_1, X_2$  - the two factors which influence the response

$B_0$  - the assumed intercept of the simulation model

$B_1, B_2$  - the assumed slope coefficients of the simulation model

$\hat{Y}$  - the estimated response surface of Y

$b_0$  - the estimated intercept of  $B_0$

$b_1, b_2$  - the estimated slope coefficients of  $B_1, B_2$

effects,  $(5*4)/2 = 10$  two-factor interactions,  $(5*4*3)/6 = 10$  three-factor interactions,  $(5*4*3*2)/24 = 5$  four-factor interactions, and 1 five-factor interaction. It becomes very difficult to describe to a manager or even another analyst the difference between a five-factor interaction and just plain error within the model. To estimate a first-order model the objective is to estimate the overall mean plus estimate only the linear effects of each of the factors. If the analyst is willing to accept the loss of information about higher-order interactions much fewer experimental runs will be adequate. The fractional  $2^k$  designs do just that.

Outstanding references on the fractional  $2^k$  designs include Box and Hunter's pair of articles "The  $2^{(k-p)}$  Fractional Factorial Designs: Part I and Part II" (11,12) and Cochran and Cox's Experimental Designs (16). If just a listing of designs is needed, Appendix A to Chapter B of Experimental Designs (16) lists a few. If a more complete listing is needed the government publication, Fractional Factorial Experiment Designs for Factors at Two Levels (22), contains fractional designs for up to 16 factors.

In Box and Hunter's pair of articles, they describe the fractional  $2^k$  factorial designs needed to estimate a first-order model as Resolution III fractionals. They state that designs of Resolution III are designs "in which no main effect is confounded with any other main effect, but main effects are confounded with two-factor interactions and two-factor interactions with one another." (11:319) What

this means is that effects due to main factors can be separated from one another, but that, as a result of reducing the number of runs taken, all the other possible effects are mixed with the main effects and each other. If the analyst, at least for an initial experiment, can assume interactions to be negligible the amount of runs of the simulation model is drastically reduced. For example, in a six-factor experiment for the full factorial, 64 runs are required; yet, the resolution III fractional design is 1/8 of the full design requiring only eight runs. This reduction in number of runs required is a significant savings of computer time. If an experimenter, because of the variability in his/her simulation model, desires to take five repetitions per design point in order to better estimate what the real-world system's response would be, the savings for six factors would be 48 runs versus 384 runs.

Designs which are used to fit second-order models are  $3^k$  full factorial designs, fractional  $3^k$  factorial designs, simplex designs, central composite designs, and a fairly recent set of designs derived in the Box and Behnken paper in 1960. (7) The  $3^k$  full factorial, fractional  $3^k$  factorial, and central composite designs are relevant to this research effort.

The response surface literature suggests using central composite designs, because in an experimental series the central composite designs can be used without reobtaining all the design points. (4,10,13,14,16,26,30,36) In general, the

central composite design is formed by combining three parts. One part is the experimental points adequate to fit the main effects of factors and all two-factor interactions (a  $2^k$  full factorial or a resolution V fractional factorial). The second part is added axial (or star) points, and the final part is the added center points. The resolution V fractional  $2^k$  factorial designs are defined as designs "in which no main effect or two-factor interaction is confounded with any other main effect or two-factor interaction but two-factor interactions are confounded with three-factor interactions." (11:319) These designs, as well as the others used in this program, will be detailed in the section on design generation of the program description chapter (Chapter IV). The important aspect of central composite designs is that, if a first-order design has already been run, only those extra runs included in the central composite design but not included in the first-order design need to be run.

The full  $3^k$  factorial and fractional  $3^k$  factorial designs are similar to the full  $2^k$  factorial and fractional  $2^k$  factorial designs. In the  $3^k$  series each of the factors is taken at three levels. For the full designs, the number of runs required in order to gain observations at each of the factor level combinations increases by three times for each factor added. For two factors, nine runs are required; for three factors, 27 runs are required; for four factors, 81 runs are required; for seven factors, 2,187 runs are required. The number of parameters to be estimated is only

one (for the intercept term) plus the number of factors (for the linear effect coefficients) plus the number of factors again (for the squared effect coefficients) plus the number of factors minus one times the number of factors divided by two (for all the two-factor interaction coefficients) (i.e.  $1+k+k+(k(k-1)/2)$ ). Even for seven factors, the total number of coefficients needed to be estimated is only 36, but 2,187 runs must be made, each a certain number of times as deemed necessary by the analyst.

The alternative to using the full  $3^k$  factorial design is to use the fractional  $3^k$  factorial designs. The smallest fraction that can be used is one which estimates main effects and all two-factor interactions. An example of the comparison between number of runs required is for seven factors. The full factorial requires 2,187 runs, while the  $1/9$  fractional design requires 243 runs -- a significant reduction in the number of runs required. An excellent reference for fractional  $3^k$  designs is the government publication by Connor and Zelen, Fractional Factorial Experiment Designs for Factors at Three Levels (17). These designs, the full  $3^k$  and fractional  $3^k$  designs, were stated to be inferior to the central composite designs for estimating the squared coefficients. (13,14,16,26,30) Nevertheless, because these designs are so widely accepted and used in computer simulation experiments, this response surface methodology package offers them also.

The simplex designs were not recommended in the



literature, because they leave no degrees of freedom to test lack of fit, and, therefore, they were not programmed into this package. (30:119)

The designs proposed by Box and Behnken were not included in this package. (7) To date, these designs have not been used in the application literature for stochastic simulation experiments. However, at a later date this set of designs should be added. At this time, though, since the user has the option to input his/her own design, these designs can be used with that option. Following the same line of reasoning, the user who is knowledgeable about experimental designs may want to confound certain effects and not others. He/she again has the option of inputting his/her own design. There exists much literature on confounding schemes in experimental designs, some of which is included in the bibliography. These references offer the user interested in these types of designs a starting point.

To summarize, the designs offered by this package are the full  $2^k$  factorial, the fractional  $2^k$  factorial, the full  $3^k$  factorial, the fractional  $3^k$  factorial, the central composite design, and the user input design option.

#### Response Surface Methodology

Response surface methodology, RSM, was initially developed and described in a paper by Box and Wilson, published in the Journal of the Royal Statistical Society in 1951 (14). According to the authors, their paper came about

as a result of a study by a chemist and statistician extending over a period of a few years. To quote Box and Wilson, development of RSM "has come about mainly in answer to problems of determining optimum conditions in chemical investigations, but we believe that the methods will be of value in other fields where experimentation is sequential and the error fairly small." (14:1) Their problem was to develop the best method to obtain optimum conditions by the process of sequential experimentation.

Two excellent texts containing chapters on response surface methodology are Experimental Designs by Cochran and Cox (16) and a book on the design of experiments authored by a team of Imperial Chemical Industries' chemists and statisticians (10). The most recent and thorough book on RSM was written by R. H. Meyers in 1971, titled Response Surface Methodology. (30) Meyers' book devotes itself to all the theoretical background needed in experimental design and regression analysis before explaining in detail the aspects of response surface methodology. Some superb articles written on RSM are included in the bibliography (4,8,11,12,13,24,26). If a comprehensive background is desired, Hill and Hunter published "A Review of Response Surface Methodology: A Literature Survey" in Technometrics in 1966. (26) This article will give the reader a good starting point for literature about RSM.

Before continuing, some definitions need to be stated. These definitions are taken from The Design and Analysis of

Industrial Experiments (10); nevertheless, the terms have comparable meaning across all the literature. The factors are the terms which influence the response. The response is the result of a reaction of factors. The response function is a mathematical function which describes the relationship between the factors and the response. And the response surface is the visual relationship (geometric representation) between the response and the factor levels. (10:496) Figure 1 is a two-dimensional representation of these terms and Figure 2 is an illustration in three dimensions.

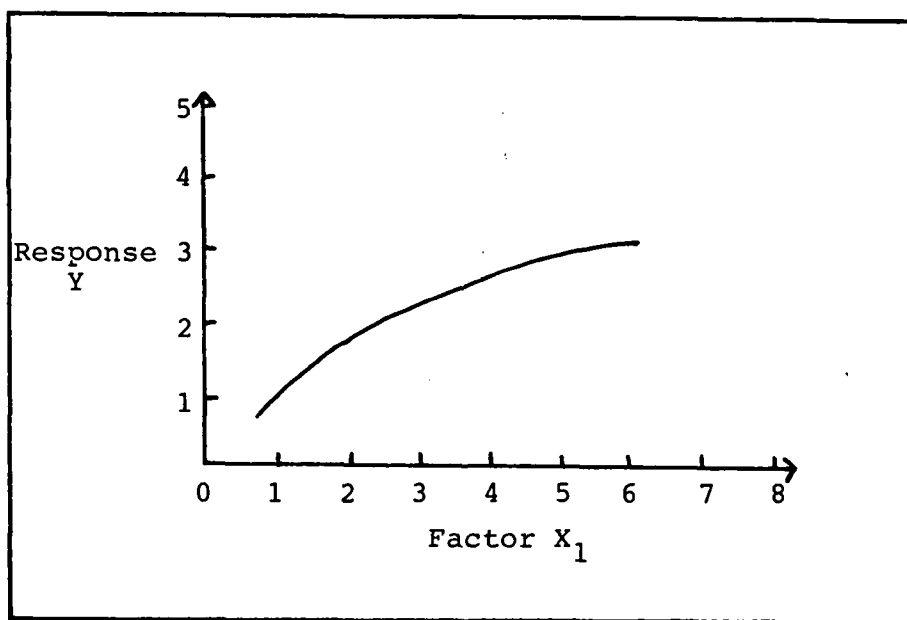


Figure 1. Response Observed for One Factor

Figure 1 shows a response surface for one factor,  $X_1$ . The response,  $Y$ , is a function of the level of  $X_1$  chosen. Therefore, the response function could be written as  $Y=f(X_1)$

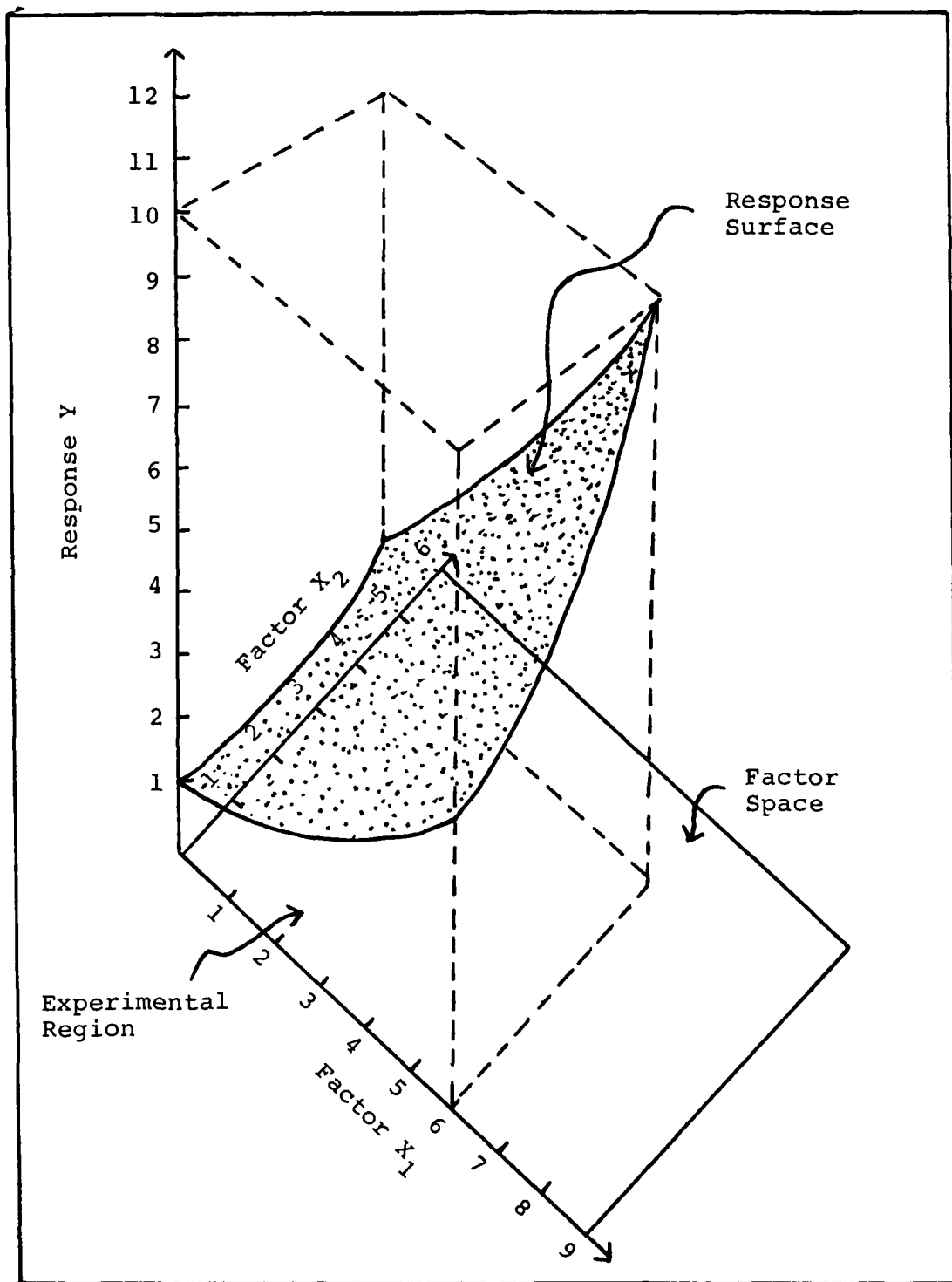


Figure 2. Response Surface Dependent Upon Two Factors and Their Interaction

where  $f(X_1)$  is the defining mathematical relationship between  $X_1$  and  $Y$ . For example, the relationship could be:

$$Y = B_0 + B_1X_1 + B_{11}X_1^2.$$

In Figure 2, the response is dependent upon two factors,  $X_1$  and  $X_2$ . More importantly, the response surface illustrates another concept, that of factor dependence. Factor dependence is the interaction between factors. The interaction in this figure is positive; in other words, there is synergism between factors  $X_1$  and  $X_2$ . The cooperative action of these factors produces a response that is greater than the sum of the responses taken independently. For example, the response function for Figure 2 could be:

$$Y = B_0 + B_1X_1 + B_2X_2 + B_{11}X_1^2 + B_{22}X_2^2 + B_{12}X_1X_2$$

where the term  $B_{12}X_1X_2$  represents the positive interaction effect.

Also illustrated in Figure 2 is the concept of experimental region. The factor space is the region of all possible factor combinations. The experimental region is that region of the factor space corresponding to factor combinations of potential interest. Also in the previous hypothetical equations, the coefficients of the linear terms represent the slope of the plane in the direction of their respective variables. The coefficient of the interaction term represents the level of interdependence between the two factors. And the coefficients of the squared terms account for the degree of curvature in the response surface due to their respective factors. A common sense conclusion is that

"as larger (experimental) regions of the factor space were considered, so polynomials of higher degree would be needed to provide a reasonable approximation to the response surface." (10:500)

Response Surface Methodology is based on a few fundamental assumptions. As listed in Meyers' text, they are:

1. A structure  $Y=f(X_1, X_2, \dots, X_k)$  exists and is either very complicated or unknown. The variables involved are quantitative and continuous.
2. The function  $f$  can be approximated in the region of interest by a low-order polynomial (either first-order or second-order).
3. The independent variables  $X_1, X_2, \dots, X_k$  are controlled in the observational process and measured with negligible error. (30:62)

Accepting these assumptions, as previously stated, the main objective is that the experimenter is concerned with elucidating certain aspects of a fundamental relationship  $Y = f(X_1, X_2, \dots, X_k)$  connecting a response,  $Y$ , with levels of a group of  $k$  quantitative variables or factors,  $X_1, X_2, \dots, X_k$ . (4:16) In "The Exploration and Exploitation of Response Surfaces: Some General Considerations and Examples", Box stresses the need for this type of investigation.

Approximate determination of the local surface and exploitation of the local factor dependence is essential to further progress. The provision of methods for doing this is thus extremely important. The advantage to the experimenter in using such methods is not merely that fewer experiments are required to attain a given result which could ultimately have been reached by traditional methods, but that a result can be obtained that could not have been got by such methods. (4:28)

In other words, if the one-factor-at-a-time method is used,

there would be no way to generate the function for  $Y$  depending upon all the factors. It would not be possible to gain information about the factor interdependencies existing within the complex system. Plus, the one-factor-at-a-time method requires many more observational runs; and, as previously stated, limits the amount of information about the system which can be obtained.

To reiterate, following the acceptance of the basic assumptions, response surface methodology is basically a combination of statistical experimental design and regression analysis applied in an iterative process, if necessary.

The next hurdle is to decide what type of experimental design to use. In Box and Draper's "A Basis for the Selection of a Response Surface Design" (8), the authors discuss, in great detail, the requirements that a response surface design should possess. Another good article to read on this subject is Box and Hunter's "Multi-Factor Experimental Designs for Exploring Response Surfaces". (13) The general problem is choosing a design such that the polynomial  $\hat{Y}=f(X_1, X_2, \dots, X_k)$  in the  $k$  continuous variables fitted by the method of least squares most closely represents the true function  $Y=f(X_1, X_2, \dots, X_k)$  over some "region of interest" in the factor space. Subject to this representation, there is a high chance that inadequacy of  $\hat{Y}$  to represent  $Y$  will be detected. Without going into the theoretical detail of the article, the authors state that when the observations are subject to error, discrepancies

between the fitted polynomial and the true function occur due to two reasons:

1) error due to sampling (more commonly called variance error), and

2) error due to the inadequacy of the polynomial,  $\hat{Y}$ , to exactly represent  $Y$  (more commonly called bias error).

(8:622)

Suitable requirements for response surface designs as stated in the literature (4,8,10,13,14,16,30) are:

1) the design should allow the graduating polynomial of chosen degree to represent the true function as well as possible within the region of interest;

2) It should allow a check to be made on the representational adequacy of the polynomial;

3) It should not contain an excessively large number of experimental points;

4) It should lend itself to "blocking"; and

5) It should form a nucleus from which a satisfactory design of higher order could be built in case the polynomial of degree chosen proved representationally inadequate.

Keeping these requirements in mind, designs appropriate for fitting first-order models are illustrated next. The literature states that, "the experimental plan or design which minimizes the variance of the coefficients is a design which is orthogonal." (30:109) If the design matrix  $X$  is orthogonal, then  $X'X$  ( $X$  transpose times  $X$ ) equals a diagonal matrix. Table II is an illustration.



TABLE II  
Example of Orthogonality

$$X = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

X is 8 x 4  
number of rows = 8

$$X' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}$$

X' is 4 x 8

$$X'X = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix}$$

X'X is 4 x 4  
8 along diagonal

The orthogonal designs most often used for fitting first-order models are the full  $2^k$  factorial and the fractional  $2^k$  factorial designs. These designs satisfy the requirement to minimize variance error, but what about bias error? If an experimenter is positive that the true model is first-order, then he need not worry about biasing or aliasing his first-order coefficients. However, frequently this might not be known. If a full  $2^k$  factorial is used to fit a first-order model in the presence of a second-order system, the  $B_0$  term is biased by the squared coefficients not included in the model and the linear terms,  $B_1, B_2, \dots, B_k$ , remain unbiased. Meyers states, "For this reason biasing due to higher-order terms should be considered, and a first-order design should always be constructed so that the experimenter can measure lack-of-fit of the postulated model and be able to compare this contribution with mere chance variation or pure experimental error." (30:114) The solution to this problem is to augment the center of the design with a certain number of points, usually four center points in the literature. (10,14,16,25,30) These added center points, say  $n_2$  of them, afford the experimenter  $n_2-1$  more degrees of freedom and an estimate of pure error in the experiment. From these, degrees of freedom and measurement of pure error, the experimenter can test his model for lack-of-fit due to an inadequately proposed model. For example, if a first-order model is postulated and the lack-of-fit test is significant then the experimenter concludes that there exist higher-order

terms in the system (either squared or interaction terms or both). His/her next step would be to fit a higher-order model.

Experimental designs for fitting a second-order response surface must involve at least three levels of each variable so that all the needed coefficients in the model can be estimated. The experimental design should be chosen on the basis of its relative precision in estimating the coefficients and the amount of experimental observations required. (30:126) As previously mentioned in the experimental design section, the full  $3^k$  factorial and the fractional  $3^k$  factorial designs could be used for this purpose. The drawback of these designs is that they require an excessive amount of observations. Box and Wilson, in their initial paper on response surface methodology in 1951, devised a workable alternative to the  $3^k$  series. They developed the composite designs, of which a subset is the class of central composite designs.

The central composite designs are first-order factorial designs augmented by additional points to allow estimation of the coefficients of second-order. These additional points are typically called axial or star points. Similar to the first-order designs, a desired number of center points would be added to the design to enable the experimenter to test for lack-of-fit.

Table III is an illustration of the three-factor central composite design. What is called the base part of the design

TABLE III

Example of Three Factor Central Composite Design

X =	base part of design is full 2**3 design	1	-1	-1	-1
		1	-1	-1	1
		1	-1	1	-1
		1	-1	1	1
		1	1	-1	-1
		1	1	-1	1
		1	1	1	-1
		1	1	1	1
	2 times 3 number of axial point rows	1	-1.682	0	0
		1	1.682	0	0
		1	0	-1.682	0
		1	0	1.682	0
		1	0	0	-1.682
		1	0	0	1.682
	9 added center point rows	1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0
		1	0	0	0

is the full  $2^k$  design or fractional  $2^k$  design which can estimate all linear effects and all two-factor interactions (commonly referred to as a resolution V fractional factorial). The axial part of the design allows for estimates of the squared coefficients. There are twice as many rows of these as there are factors, and they are generated as in Table III. The constant value for the axial points is chosen so that the design becomes orthogonal and rotatable. The formula for rotatability is that the constant in the axial points equals two to the power of the number of factors divided by four. Rotatable designs insure that the estimated response has a constant variance at all points which are the same distance from the center of the design. (10:195) "If there are many replications of the center point, the standard error of  $\hat{Y}$  is low at the center and increases rapidly as we move away from the center." (16:345) If only a few center points are used the opposite will occur. In Box and Hunter's paper, they suggest that the number of center points be chosen so that the standard error of the estimated response is approximately the same at the center as at all points on the circle with radius one. (16:346)

The proposed design to use for second-order models in the literature is the orthogonal rotatable central composite design. This design lends itself well to sequential experimentation. If a first-order model was fit with a full  $2^k$  design or fractional  $2^k$  design only the observations at the axial and center points would have to be taken.

## Regression Analysis

Entire college courses have been devoted to teaching the theory and application of Regression Analysis. Hundreds of textbooks have been written on the subject. It is not the purpose of this section to explain in great detail the theoretical and mathematical aspects of regression analysis; rather, this section is more for the purpose of summarizing conceptually the ideas associated with regression analysis. If a more detailed description is needed, Draper and Smith's Applied Regression Analysis (21) is an excellent reference.

In any system in which variable quantities change, it is of interest to examine the effects that some variables exert on others. Sometimes there may be a simple functional relationship between variables, but most of the time this is not true. Often there exists a relationship which is too complex to express in simpler terms. In this situation we may want to approximate this relationship by a simple mathematical function. For instance, one might choose a polynomial which contains the proper variables and which graduates or approximates the true complex function over some limited range of the variables involved. If this mathematical function is an adequate approximation, it may be examined and certain important underlying relationships and interdependencies among variables may be revealed. (21:2)

There are two types of variables in regression analysis, independent variables and dependent variables. Independent variables are those variables which can be controlled and set

to particular values or those variables which can not be controlled, but which can be noted at particular levels. These independent variables, as they change values or levels, have an effect on dependent or response variables.

The objective in regression analysis is to determine the 'best' linear (in the parameters) relationship between a set of independent variables and their associated dependent variables (refer back to Table I). The analytical technique employed to find this 'best' linear fit is called the method of least squares. This method minimizes the sum of the squared deviations about the regression line.

In matrix notation, suppose  $m$  is the number of observations and  $n$  is the number of independent variables. The experimenter wants to fit the linear relationship  $\hat{Y} = b_0 + b_1X_1 + \dots + b_nX_n + e$ . Assume that the errors are independent identically distributed normal with mean zero and variance some  $\sigma^2$ . The algorithm to determine the vector of beta estimates is:

$$XB = Y \quad [Y \text{ is } m \text{ by } 1, X \text{ is } m \text{ by } (n+1)]$$

$$X'XB = X'Y \quad [B \text{ is } (n+1) \text{ by } 1]$$

$$(X'X)^{-1}(X'X)B = (X'X)^{-1}X'Y$$

The least squares estimates of  $B$  are given by:  $b = (X'X)^{-1}X'Y$ .

A more detailed description of the actual procedure used in this program is included in the program description chapter.

#### Applications of Response Surface Methodology

Many applications of RSM have been made in the classical experimental lab situation. In this situation physical reactions are measured in a highly controlled environment. Typical areas where this situation has occurred are tool-life testing, chemistry, and food-stuffs. The literature survey by Hill and Hunter contains many of these type applications.

(26)

More pertinent to this research effort are those applications of RSM to simulation models. Unfortunately, since most of the RSM techniques are applied uniquely to each simulation model, there are not many applications published in the literature. One application which has been published was written by Hufschmidt and is titled "Analysis of Simulation: Examination of Response Surface". This application is included as a chapter in the book Design of Water-Resource Systems. (27) His stochastic simulation was a model of a simplified river-basin system. The objective of the study was to locate the optimal region for operability. He used both systematic sampling and random sampling techniques to locate this region. At the same time suboptimal regions were explored by response surface methodology to flag which variables had the most impact on net benefits. So RSM in combination with sampling techniques was used to locate the optimal region for system operability.

(27)

A recent article titled "A Variance-Reduction Strategy for RSM Simulation Studies" by Cooley and Houck was published



in 1982. They state that "the application of optimization techniques in digital simulation experiments is frequently complicated by the presence of large experimental variances." (19:303) They state that even though RSM has been applied successfully in many other experimental environments, it has not been widely accepted in simulation studies. In their article they propose using a combination of two techniques of variance reduction -- assignment of common pseudo-random number streams and the assignment of antithetic pseudo-random number streams -- in response surface methodology analyses of simulation models. To demonstrate the application and benefits of their proposed assignment procedure, they include an example of a simulation model of an inventory system. Similar to Hufschmidt's article, their main objective is to use RSM in an optimization process. They fit the initial experimental region with a first-order model, use the method of steepest ascent to direct them to a more optimal region, then refit a first-order model in the second region. As they approach the optimal region, the first-order model no longer demonstrates an adequate fit; subsequently, they fit a second-order model. Once again they proceed to a more optimal region. This iterative process continues until the optimal has been reached. (19)

In 1976, Dennis Smith wrote a response surface methodology program which was presented at the November 3-5 ORSA/TIMS Joint National Meeting. His program is titled "Automated Response Surface Methodology in Digital Computer

Simulation" and the paper that describes his program is "Optimization of a Computer Simulation Response". (36,37,38) His paper summarizes the optimum-seeking problem in simulation studies, reviews the framework of RSM, and describes his automated RSM computer program, which was developed as an alternative to manual applications of RSM in the optimization process. Basically, the program follows the same iterative procedure that Cooley and Houck's article described. First, he fits an initial experimental region with a first-order model using a full  $2^k$  factorial design or a fractional  $2^k$  factorial design. He then uses the steepest ascent procedure to move in the direction of the optimal region. When the first-order model is determined to exhibit a significant lack-of-fit, a second-order model is fit, using only the orthogonal rotatable central composite design. The final output is the estimated equation of the response function in the optimal region and the optimal value. Smith has available two versions of this program, an unconstrained version and a constrained version. In other words, if the user has certain constraints applicable to his system that are not contained within the simulation model, they can be accounted for in the optimization process. Once again, the main objective is to solve the simulation model optimization problem.

#### Summary

The purpose of this chapter was to briefly describe all

the areas required when using RSM. Hopefully, these discussions will enable the user to understand the conceptualization of RSM in simulation studies, not only from the viewpoint of optimization but also for the purpose of elucidating underlying mechanisms of the real-world system, thus, enabling the analyst to answer as many questions as possible about the system.

### III Design Considerations

Any development process involves careful consideration of all aspects which could influence the outcome. The purpose of this section is to address the initial issues which guided the developmental phase and the implementation of the response surface methodology package.

#### User Considerations

Anytime a software package is to be used by people unfamiliar with the program, special consideration within the program must be given to user interface. The programmer must be sensitive to the inexperienced programmers and users that are unfamiliar with the operating system who will desire to use the software package. The user of the program should not be required to know all the detailed theory involved or be expected to change parts of the software to be able to use it. However, if a knowledgeable user should desire to add enhancements or change some of the program limitations, he/she should be able to do so without too much trouble.

With these ideals in mind, a software package such as this should provide for understandable input. The input required should be minimal and simple. This type of requirement suggests a menu-driven package which enables the user to enter input after each question and, if the question is answered incorrectly, to try again. The input required should progress in a logical sequence so that the infrequent or less knowledgeable user will not become confused and

anxious about the purpose or order of the input needed. Complete echoes of the user's input should be displayed on the screen to strengthen the user's confidence in his/her ability to use the program. When the program is completed, the output displayed should be readable and organized. Proper labels and format should be used to ensure that the user knows exactly what each piece of output means and its significance. If all these precautions are followed, the package developed will have a much better chance of being used because the user will feel comfortable with the questions and information asked of him/her and the program output will be meaningful.

#### Hardware Considerations

This software package was developed with the desire for it to be mobile from one computer system to the next. Regardless of this underlying goal, an operating system needed to be chosen for package development and illustration. The two choices available to the author are the Cyber and the Vax 11/780. It was decided to develop the program on the Vax. For the package to be used with other operating systems, the only commands requiring change are those which open and read permanent files and those which open and create permanent files. The statements are listed and discussed in the user manual chapter.

For the experienced analyst who desires to use another regression package or statistical program instead of the one

included in the program, the RSM program creates and writes the design matrix augmented with the data observations to a permanent file. The format of this file is included in the user manual chapter, and this file can be transferred to another system which offers statistical packages or can be used by the analyst for any desired purpose.

#### Language Considerations

When choosing a computer language to program the package, thought was given to language capability and acceptability of the language. The two scientific languages possible for use were FORTRAN and PASCAL. FORTRAN is more widely used and accepted in the scientific community; thus, it was decided that FORTRAN was the language best suited to be used in the program. Additionally, since FORTRAN V (more commonly called FORTRAN 77) is well suited for structured programming, this version was selected for use in the package.

#### IV. Program Description

This chapter describes the computer program and is organized as follows: (1) Development Approach, (2) Input Requirements, (3) Experimental Design Phase, (4) Intermediate Subroutines, (5) Regression Phase, (6) Subsequent Subroutines, (7) Program Verification and, (8) Program Limitations. Appendix B contains the entire program listing.

##### Development Approach

One of the main objectives of this response surface methodology computer package is that the program be relatively easy to understand. In other words, the program flow needs to proceed in a logical sequence corresponding with problem conceptualization. Figure 3 is a flow diagram of the main program. This flow diagram illustrates the logical sequence of the computer package. First, all the required user input is initiated. Next, the program enters the design generating phase. This phase consists of the subroutines needed to generate the first-order and second-order designs available to the user -- namely, subroutines FULL2K, RES3, FULL3K, CCD, FRAC3K, and USER. The intermediate subroutines follow the generation of the design desired by the user. These subroutines obtain the simulation model responses needed to calculate the response surface estimate. They convert the design matrix into values the simulation model can accept, obtain the simulation model

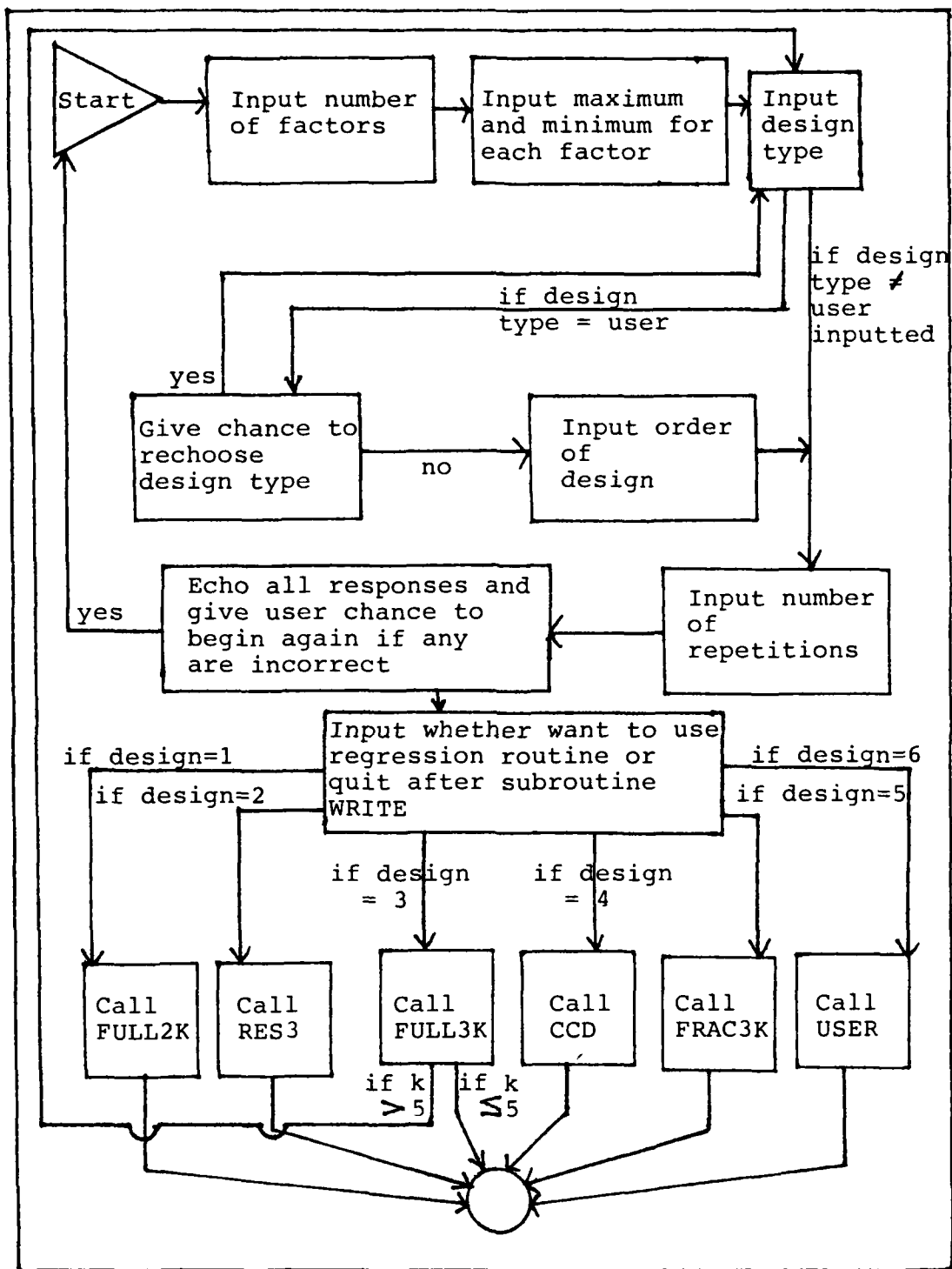


Figure 3. Flow Diagram of Main Program



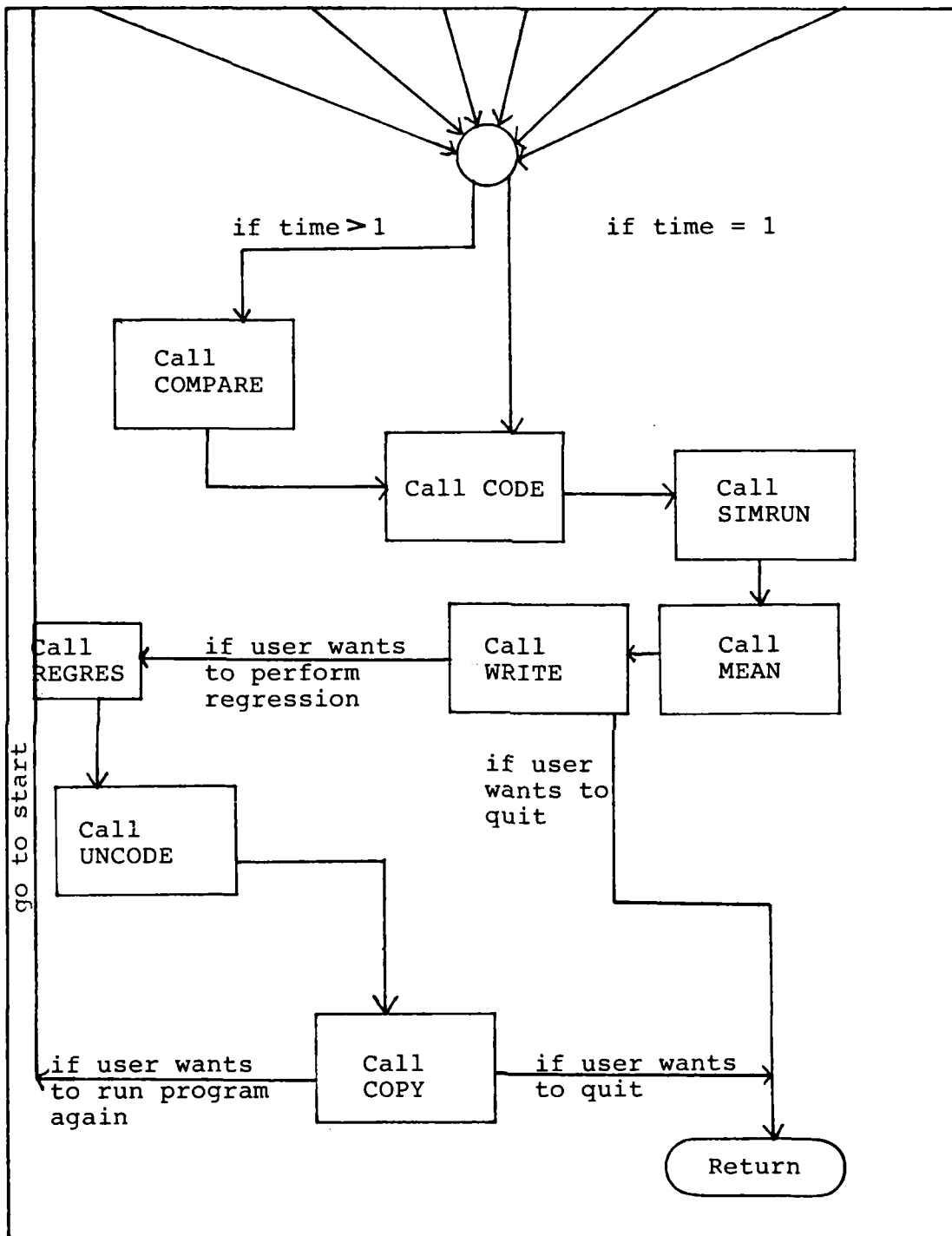


Figure 3. Flow Diagram of Main Program

responses associated with different combinations of factor levels and replicate the number of times, calculate the average simulation model responses depending on the number of replications per factor level combination, and write the design matrix augmented with the simulation model response averages to a permanent file which can be used. If the user inputs to stop after this phase, the program ends.

Otherwise, the program enters the regression phase. This phase performs the regression by the method of least squares and prints all the appropriate output such as coefficient estimates, standard errors of the estimated coefficients, an analysis of variance (ANOVA) table, and all required test statistics to evaluate the estimated response surface. The subroutines UNCODE and COPY follow the regression phase. The UNCODE subroutine decodes the coefficient estimates obtained in the regression phase. The decoded coefficient estimates are in terms of the input factor ranges rather than in terms of the factor ranges implicit in the generated design matrix. After decoding the coefficient estimates, the subroutine prints them beneath the output printed during the regression phase. Finally, the subroutine COPY, copies the design matrix and the vector of average responses obtained from the simulation model to different storage locations. If the user wants to run the program again and some of the combinations of factor levels in the design matrix are the same as previously required, the corresponding average response obtained earlier can be used again, saving the user runs of

the simulation model. This main program executive structure, flowing from one phase to the next, lessens the amount of detail the user needs in order to efficiently use the program.

#### Input Requirements

More detailed instructions on setting up the program to run with a simulation model are included in Appendix A, the user manual. Discussed in this section are the inputs required after the program is set up and ready to run. Referring back to Figure 3, all of the user input is entered first. Questions are displayed on the screen for the user to answer to satisfy the input requirements for the program. Following the main program diagram, the input requirements are: (1) input the number of factors to be used, (2) for each of these factors, input the maximum and minimum levels, (3) from the design types listed, choose the design desired, (4) input the number of repetitions desired per factor level combination, (5) input whether a mistake was made and new start is desired, and (6) input if the regression package offered by this program is desired or want to stop after average simulation model responses are obtained and use written file 'MATRIX' to perform your own analysis. If any of these inputs are incorrect, the range of possible correct inputs is displayed and the user is requested to respond again.

#### Experimental Design Phase

This section first describes each of the design generation subroutines. Following the subroutine descriptions, a comparison between the number of observations required, depending on the design type, is given. Finally, this section discusses the verification process used for the design generation phase. Appendix C contains the listing of all the designs used in this program.

FULL2K Subroutine. Figure 4 is the flow diagram for the FULL2K subroutine. The first operation is to calculate the dimensions to be used by the design matrix. The number of rows equals  $2^k$  while the number of columns equals  $k+1$ , where  $k$  is the number of factors. Next, the matrix of proper dimensions is initialized. After this, the first column of all ones is generated to be used to estimate the intercept term in the regression phase. Next, all the rest of the columns are created according to the pattern required for generating full  $2^k$  designs (refer to design listings in Appendix C). Following the generation of the full  $2^k$ , center point rows are added to allow for a test of lack-of-fit of the proposed model which estimates the response surface implicit in the simulation model. The observations obtained at the center points enable an estimate of pure error to be obtained. The remaining amount of residual error is attributable to lack-of-fit of the proposed model due to higher-order terms or interaction terms not included. These calculations are discussed in further detail in the regression phase section of this chapter. After the

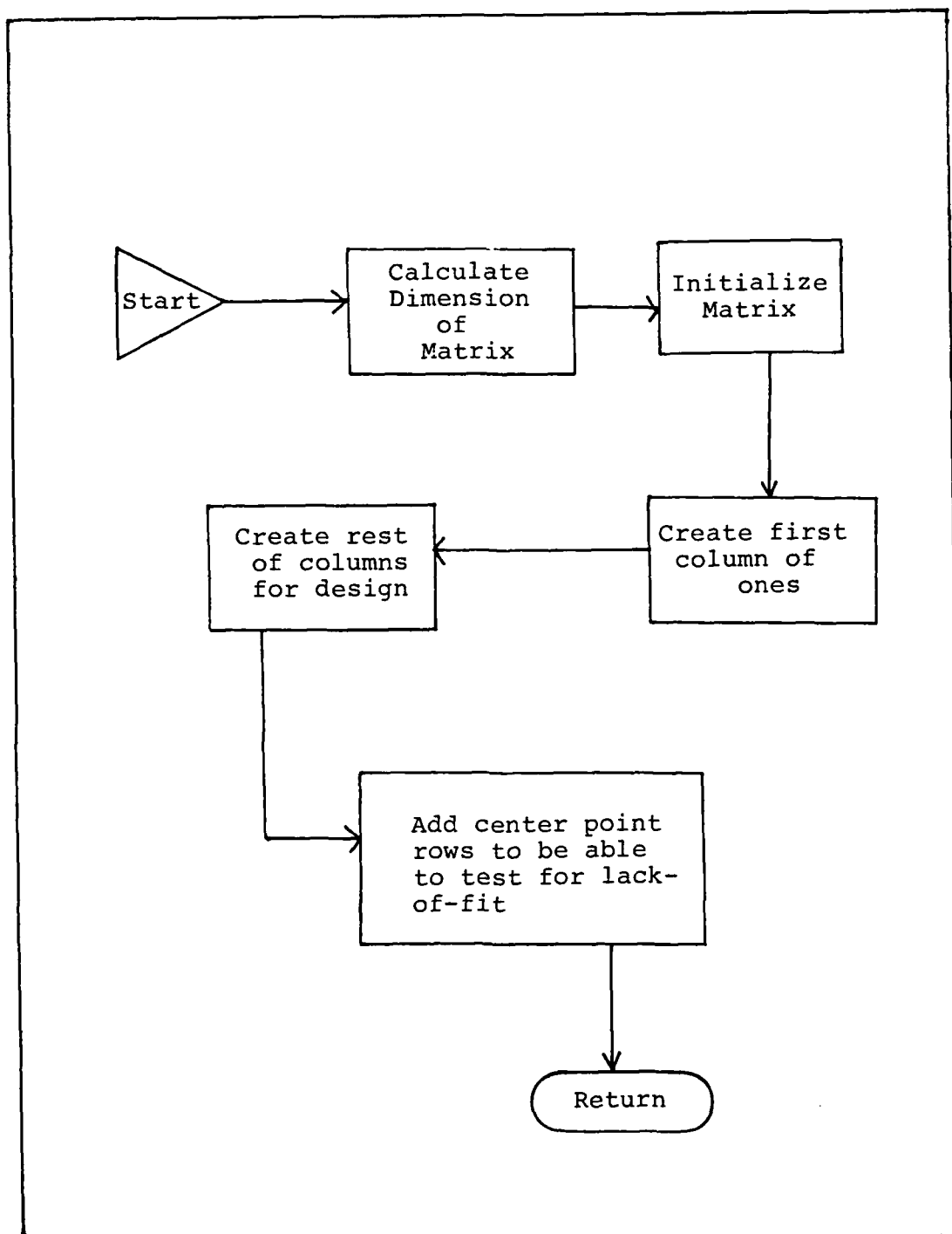


Figure 4. Flow Diagram of FULL2K Subroutine

center point rows are added, the generation of the full  $2^k$  design needed is complete.

RES3 Subroutine. A flow diagram of the RES3 subroutine is given in Figure 5. In general, this subroutine generates the resolution III fractional  $2^k$  factorials required from rows of a 1/16th replication of the full  $2^9$  design matrix. All of these designs for two to nine factors are listed in Appendix C with their corresponding references. To generate these designs, first the file 'RESTHREE' is opened. This file contains the 1/16th fractional  $2^9$ . If the number of factors input are two or three, there is no resolution III fractional. Therefore, for the number of factors equal to two or three, the subroutine calls the FULL2K subroutine to generate the design matrix and then returns to the main program. If the number of factors is greater than three, the subroutine copies the applicable rows from file 'RESTHREE' into the design matrix. After all the rows are added to the resolution III design, four center point rows are added to make it possible to give an estimate of pure error. These center point rows complete the design generation.

FULL3K Subroutine. Figure 6 is the flow diagram of the FULL3K subroutine. This subroutine generates the full  $3^k$  design matrix needed, depending on the input number of factors. If the number of factors is greater than five, this subroutine is not allowed to be used. The user is informed to use either the central composite design or the fractional

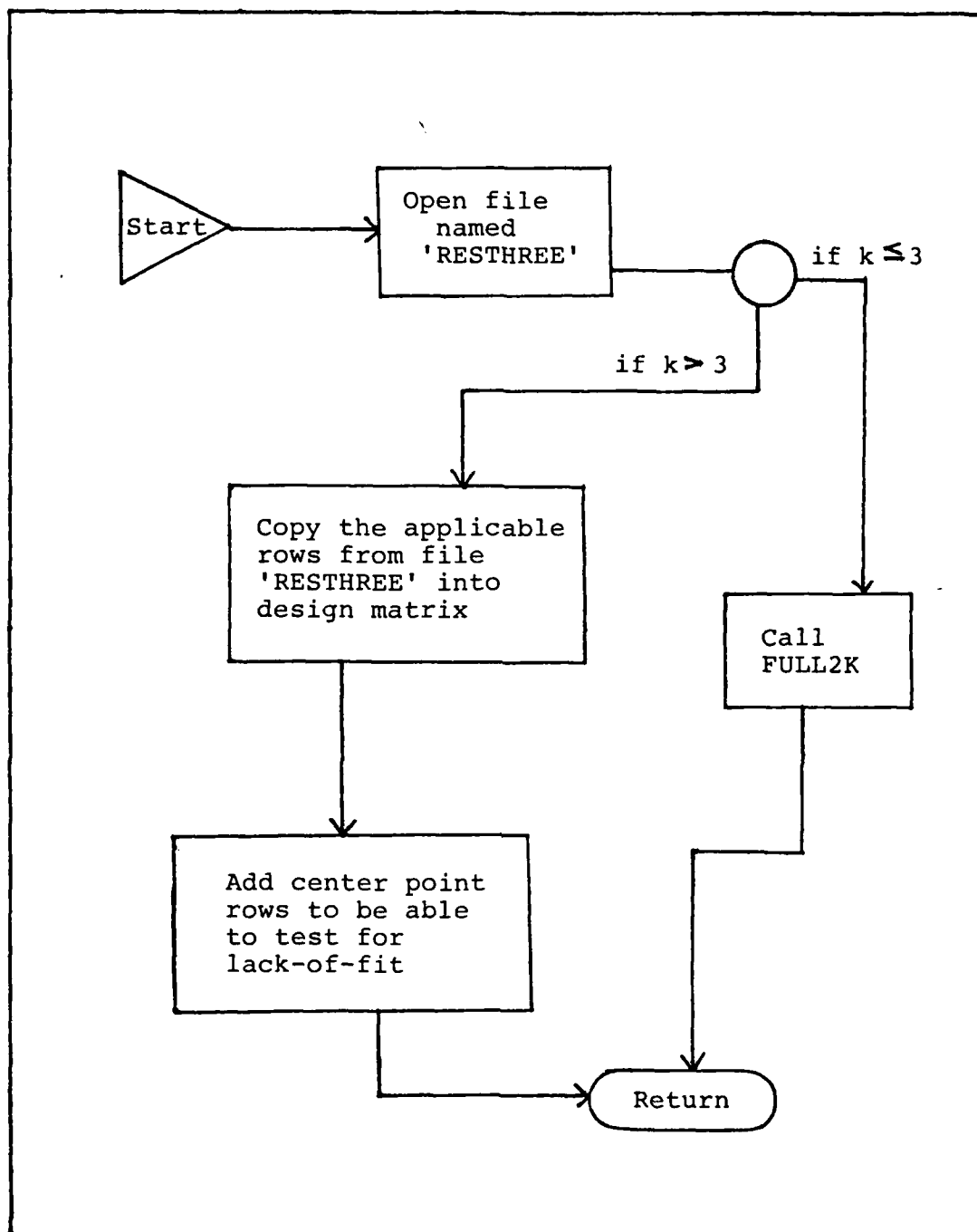


Figure 5. Flow Diagram of RES3 Subroutine

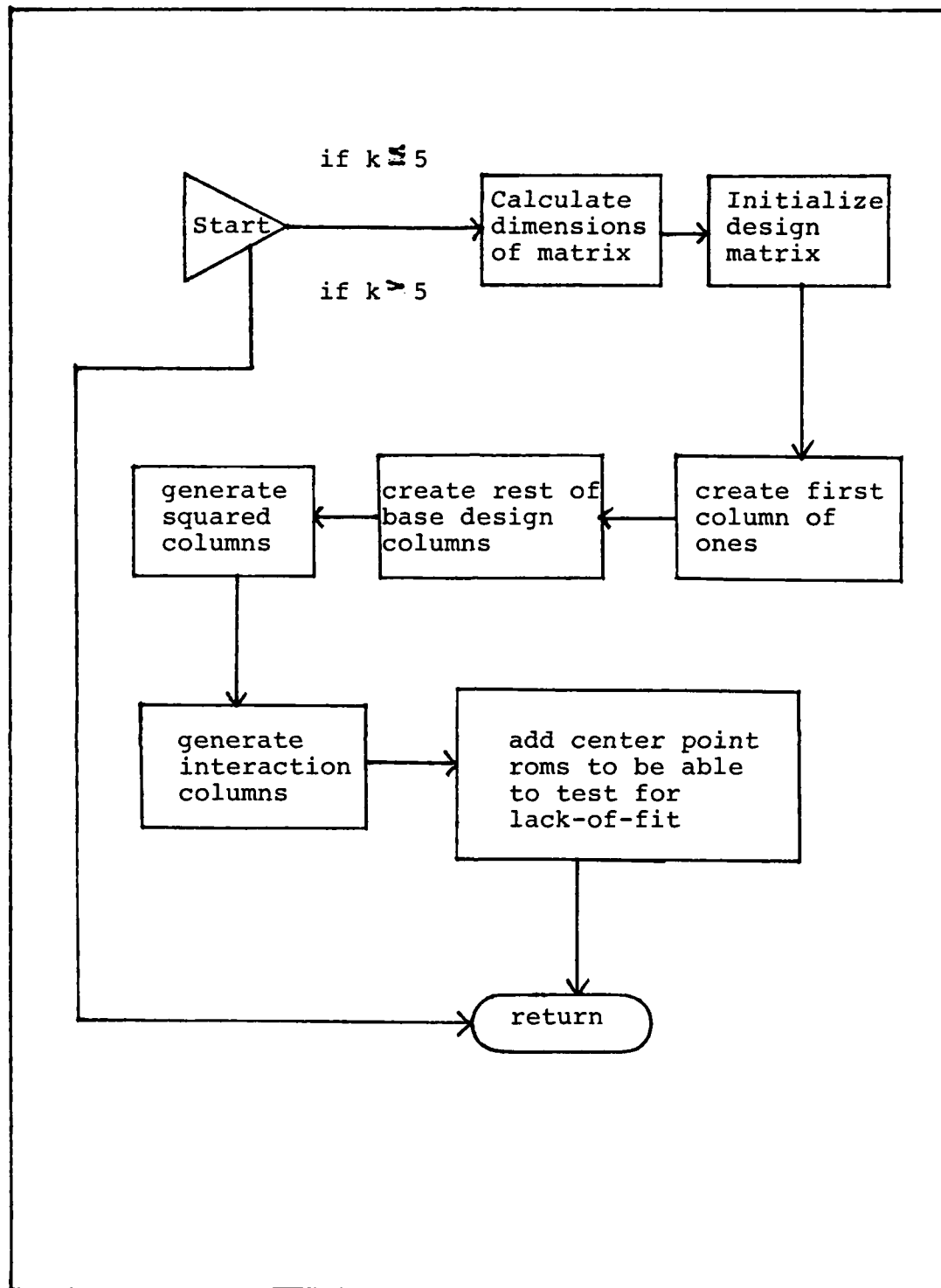


Figure 6. Flow Diagram of FULL3K Subroutine



$3^k$  design offered, and is permitted to reselect the design type desired. Also, if the number of factors is greater than five, the user is informed where to change this limitation, if desired. If the number of factors is less than or equal to five, the routine starts to generate the design matrix needed. First, the dimensions of the matrix are calculated. the number of rows equals  $3^k$  and the number of columns equals  $1+2k+(k(k-1)/2)$ . One column is for the intercept,  $k$  columns are for the linear effects of the factors,  $k$  columns are for the factor squared effects, and  $k(k-1)/2$  columns are for all the two-factor interactions. Similar to the generation of the full  $2^k$  designs, the matrix is initialized next, then, the first column of ones is generated, followed by the rest of the design, generated according to the pattern for  $3^k$  designs (refer to Appendix C for the design listings). After the generation of the base design, the columns to estimate squared terms and interaction terms are formed. These are formulated by multiplication of the appropriate columns. When these columns are completed, four center point rows are added so pure error of the proposed second-order model can be estimated.

CCD Subroutine. The flow diagram for the central composite design subroutine is pictured in Figure 7. Basically, this subroutine generates the ccd designs in three stages. The first stage generates what is called the base part of the design, the resolution V fractional factorial needed to estimate linear and all two-factor interaction

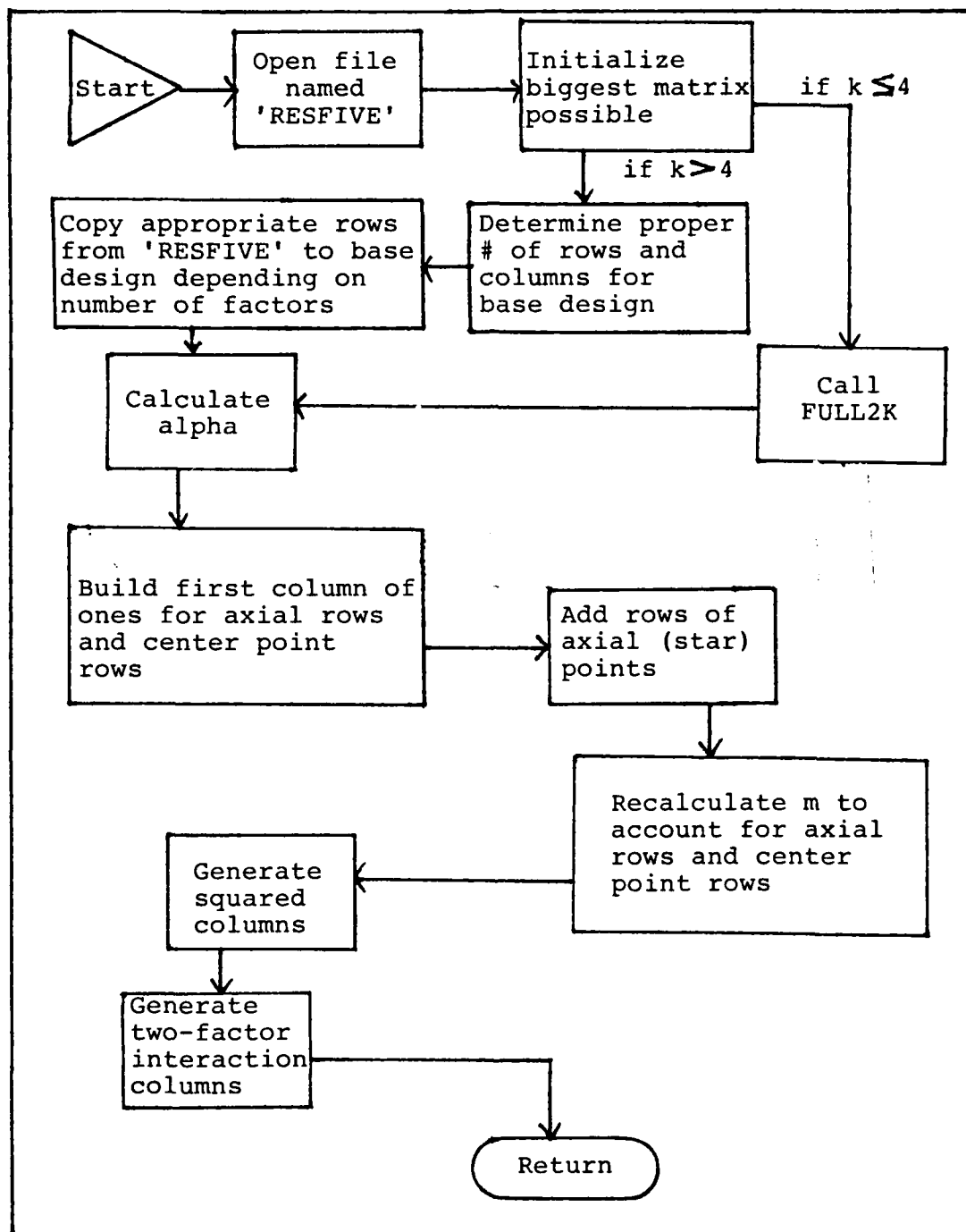


Figure 7. Flow Diagram of CCD Subroutine

terms. Next, the rows of the axial (star) points needed to estimate the squared terms are added. The final stage adds the desired number of center points to estimate pure error, while at the same time, retaining orthogonality and rotatability. Referring to Figure 7, the subroutine first opens the file 'RESFIVE' and initializes the biggest matrix needed. If the number of factors is less than or equal to four, the subroutine calls the subroutine FULL2K to generate the base part of the design, since there is no resolution V fractional for four or less factors that can estimate all linear and two-factor interaction terms. Once this full  $2^k$  factorial is generated, for four or less factors, the subroutine goes directly to the next stage, adding the axial rows. For five or more factors, the subroutine copies the proper rows (depending on the number of factors) from the file 'RESFIVE', which is a 1/4th replicate of a full  $2^9$ . These rows will make up the resolution V base design part.

The next stage is adding the axial rows needed to estimate the squared effects. The axial rows, as discussed in Chapter 2, are formed according to the following pattern for three factors:

$$\begin{array}{ccc} -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & \alpha \end{array} .$$

The number of axial rows is twice the number of factors. The  $\alpha$  is chosen so that the central composite design retains the

desired properties, orthogonality and rotatability. Specifically,  $\alpha = 2^{k/4}$ . For each half replicate, one would be subtracted from the numerator. For example, when k equals five, a 1/2 replicate is used for the base design, thus  $\alpha = 2^{(5-1)/4}$ . Table IV lists the appropriate  $\alpha$ -values for two to nine factors. After the  $2k$  axial rows are added, the center point rows are added. Table IV lists the proper number of center point rows needed for two to nine factors, dependent upon the size replicate that is used as the base part of the design.

This program uses the smallest replicate of the full  $2^k$  design that still allows estimation of all linear and two-factor effects. The fractions used in this program are annotated in Table IV. The proper number of center points is crucial to retaining orthogonality and rotatability, and Table IV shows how the required number of center points changes depending on the replicate used as the base design. The calculation of the squared and interaction columns follows the generation of the center point rows. The code which generates these columns is identical to that used in the FULL3K subroutine.

FRAC3K Subroutine. Figure 8 is the flow diagram for the FRAC3K subroutine. If  $k \leq 4$ , the subroutine calls the FULL3K subroutine, since no fraction of the full  $3^k$ , for  $k \leq 4$ , exists which can estimate all linear, squared, and interaction terms. If  $k \geq 5$  the number of rows are determined. Next, the first column of ones needed to estimate the intercept is

TABLE IV

Rotatable/Orthogonal CCD Designs (13:227)

k	2	3	4	5 ( $\frac{1}{2}$ )	6 ( $\frac{1}{2}$ )	7 ( $\frac{1}{2}$ )	8 ( $\frac{1}{2}$ )	*8 ( $\frac{1}{2}$ )	9 ( $\frac{1}{2}$ )
factorial pts	4	8	16	16	32	64	64	128	128
$n_a$	4	6	8	10	12	14	16	16	18
$n_o$	8	9	12	10	15	22	20	33	31
N total	16	23	36	36	59	100	100	177	177
$\alpha$	1.414	1.682	2.0	2.0	2.378	2.828	2.828	3.364	3.364

\* Not offered in this program

k - number of factors

 $n_a$  - number of axial points $n_o$  - number of center points $\alpha$  - calculated alpha to use

N- total number of points in design

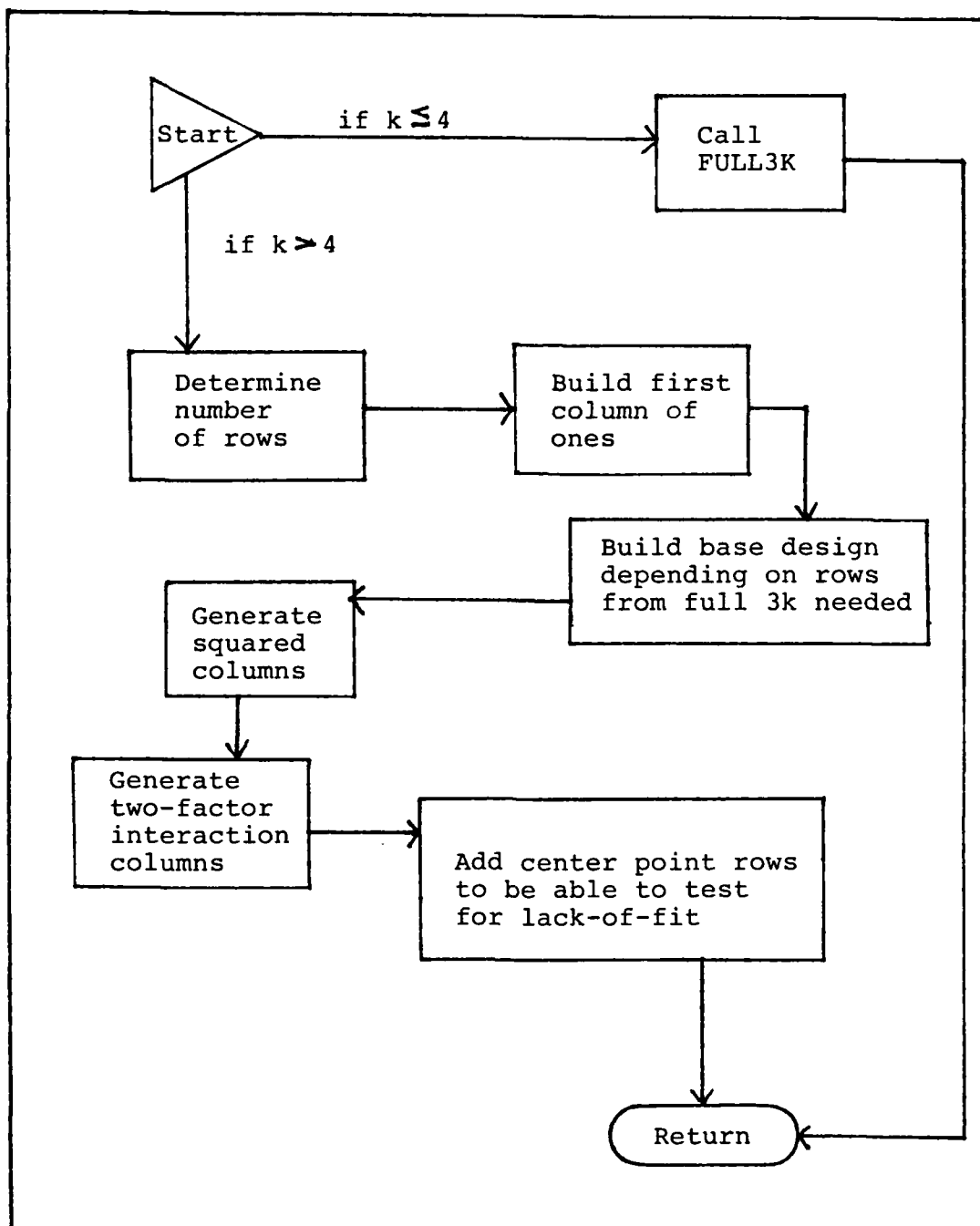


Figure 8. Flow Diagram of FRAC3K Subroutine

generated. After generating this column of ones, the next  $k$  columns are generated for each row depending on the rows included from the full  $3^k$  design. Refer to Appendix B, the program listing, for the algorithm used to generate the base design. After the base design is generated, the columns required to estimate squared and two-factor interaction effects are calculated in the same manner as they were in the FULL3K and CCD subroutines. The last procedure to complete the fractional  $3^k$  design, is to add the center point rows to enable a pure error estimate to be made.

USER Subroutine. The flow diagram for the USER subroutine is shown in Figure 9. First, this subroutine prints directions on how the user should input his/her desired design. The next input required is the number of rows and the number of columns. Following this input, the user inputs the design by rows according to the prompt messages. After the entire design is input, the program prints an echo check for the user to verify his/her design input. The subroutine then returns control of the package to the main program.

Comparison of Observations Required by Designs. Each of the designs offered by this program has its advantages and disadvantages. The biggest problem for simulation model experimental designs is the number of observations required. In a complex simulation model, the experimenter wants to gain as much information as possible with the least possible expenditure of time and effort. The more variable the

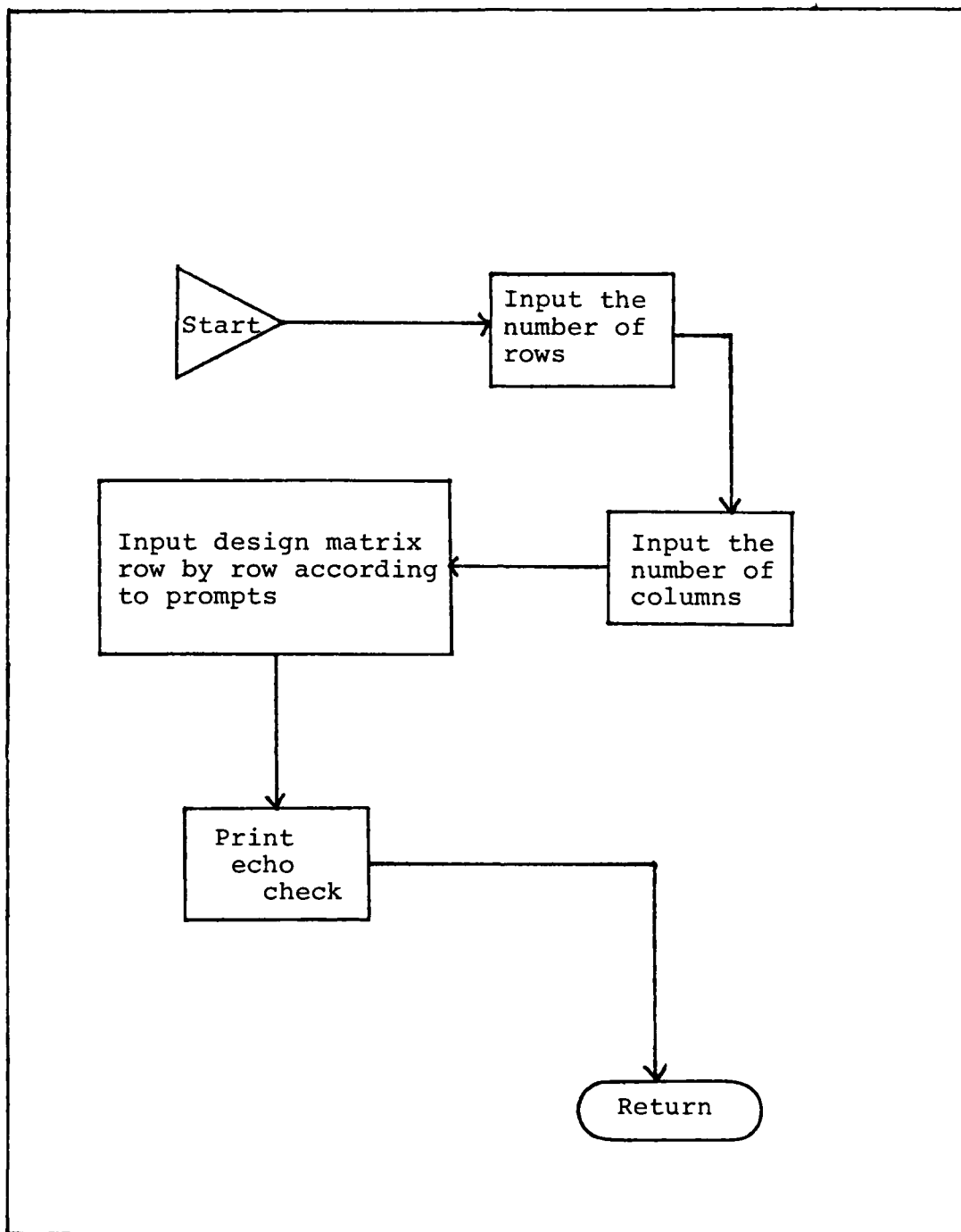


Figure 9. Flow Diagram of USER Subroutine



simulation model, the more repetitions per design point that will have to be taken. Table V lists the required number of mean observations, dependent upon the number of factors and design type chosen. The amount of care that should be used in selecting the design type is directly proportional to the number of factors used in an experiment. Suppose a simulation model has significant variation in its observations as a result of many stochastic processes involved, thus five replications need to be made per observation. A first-order design is needed and there are eight factors to be tested. To run this RSM program and use the full  $2^8$  design would require 1280 separate simulation runs. Whereas, to use the smallest fraction of the full  $2^8$  needed to estimate linear effects would require only 80 runs.

For the second-order designs, the differences between the number of runs required by design types is much greater. For this reason, the full  $3^k$  design is not allowed to be selected for a number of factors greater than five. The user needs to give careful consideration to design type and number of replications desired before input of the design type desired.

Verification of Design Generation Phase. The design generation phase of this program was verified by two processes. All the designs offered by this program are nearly orthogonal. For a design to be orthogonal there are three requirements:

TABLE V

Number of Points Needed by Design Type

k	2	3	4	5	6	7	8	9
*full2k	4	8	16	32	64	128	256	512
*res3	4	8	8	8	8	8	16	32
**full3k	9	27	81	243	729	2187	6561	19683
**ccd	16	23	36	36	59	100	100	177
**frac3k	9	27	81	81	243	243	243	243

\* first-order designs

\*\* second-order designs

full3k not offered for  $k \geq 6$

- 1) The dot product of any two columns must equal zero,
- 2) The sum of the squares of column entries for any column must be equal to the total number of rows, and
- 3) The sum of the column entries for any column must equal zero. (30:109)

The algorithms that were used to generate all the offered designs (discussed in the previous sections) were developed in such a way that, if an error was made in generating a design for a particular number of factors, an error would also be made in at least one other design in the same set, but for a different number of factors. It was determined that since several of the designs would be incorrect if the design generation phase proved to have an error that an adequate check would be to verify the requirement that the dot product of any two columns is equal to zero. The exception to this rule is that in the second-order designs, the dot product of the squared columns and the column of ones used to estimate the intercept is not equal to zero. However, for any of the first  $k+1$  columns the dot product is equal to zero. Thus, if a design is generated correctly an adequate check is that the sum of all possible dot products of the  $k+1$  columns would equal zero. If any dot product was not equal to zero, the sum would not equal zero and the design generated would be incorrect. To check this sum of dot products, a dot product check program was written to use with any of the designs for the  $k+1$ st columns. When this program was run with the generated designs, the sum for each

checked correctly. To check the remaining columns of the second-order designs, the multiplication of proper columns was evaluated and all of the remaining columns for the second-order designs checked out correctly.

The second process used for verification of the design generation phase involved a significant effort. All the generated designs from the sets full  $2^k$ , fractional  $2^k$ , full  $3^k$ , and central composite design for two to nine factors were checked by hand. All these generated designs checked out. Since the fractional  $3^k$  set contained such large designs a complete check by hand was not feasible. However, spot checks were made throughout the fractional  $3^k$  design set for two to nine factors. The spot checks revealed no errors.

These two processes were used in conjunction with one another to verify the program's design generation phase.

#### Intermediate Subroutines

There are five intermediate subroutines. They are: (1) COMPAR, (2) CODE, (3) SIMRUN, (4) MEAN, and (5) WRITE.

COMPARE Subroutine. Figure 10 is the flow diagram for the COMPARE subroutine. Basically this subroutine compares the generated design matrix for this program run with the previously used generated design matrix. If two rows of both design matrices are identical, and have not been identified before in this subroutine, the average response obtained from running the simulation model previously can be used again. The identified average response is then copied into the

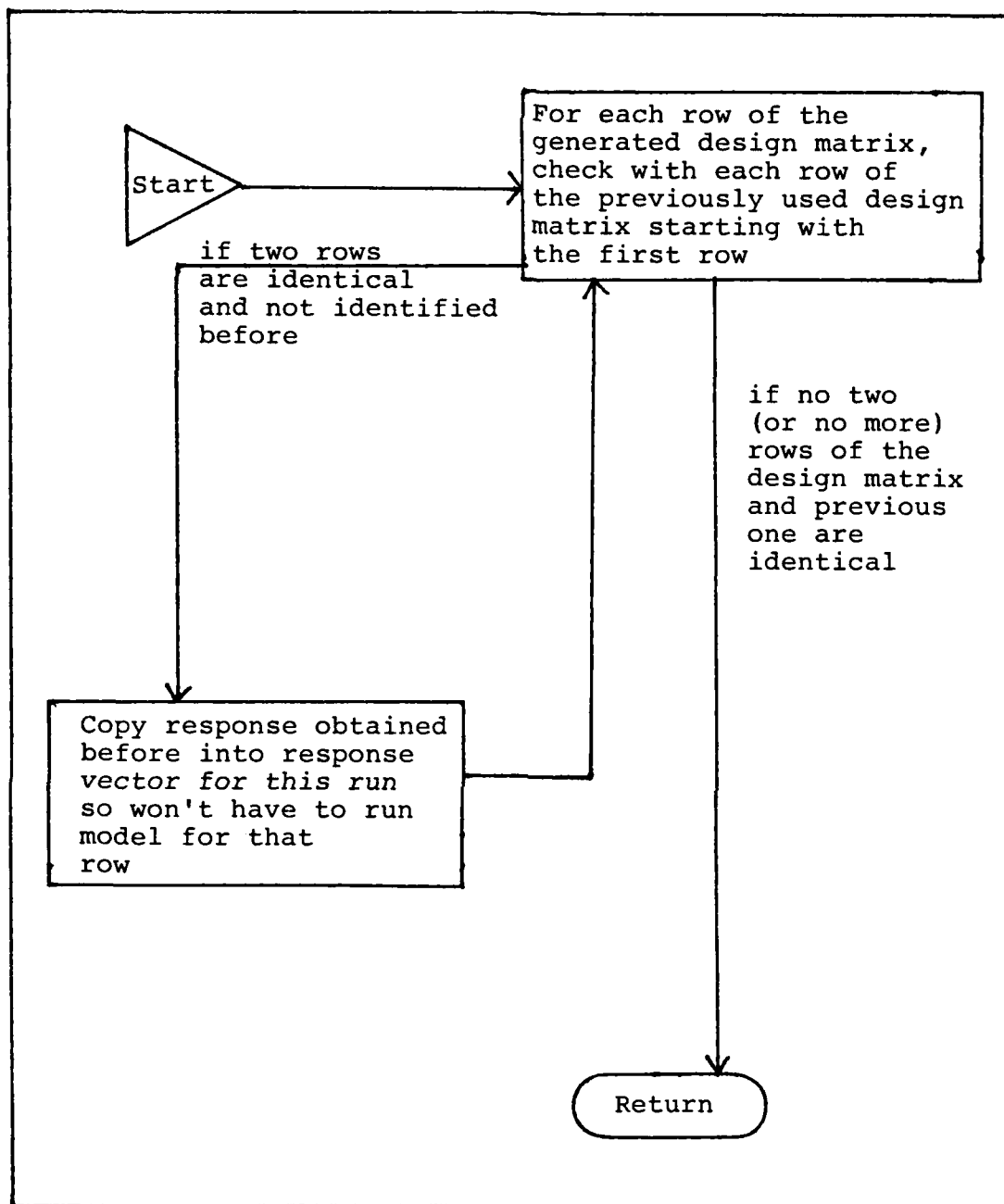


Figure 10. Flow Diagram of COMPAR Subroutine

corresponding average response vector for the row which does not have to be run again. After every comparison is made, the subroutine returns.

CODE Subroutine. The flow diagram for this subroutine is depicted in Figure 11. The purpose of the CODE subroutine is to code the design matrix into a matrix that has the factors at the levels needed for the simulation model. First, the ranges and averages for each factor are calculated according to the formulas:

$$\text{range}(\text{factor}) = \text{maximum}(\text{factor}) - \text{minimum}(\text{factor})$$

$$\text{ave}(\text{factor}) = (\text{maximum}(\text{factor}) + \text{minimum}(\text{factor}))/2.$$

Then the new elements for the coded matrix are calculated by the formula:

$$\text{new element} = \text{old element} * \text{range}(\text{factor})/2 + \text{ave}(\text{factor}).$$

Following the coding, the subroutine returns to the main program.

SIMRUN Subroutine. Figure 12 is the simple flow diagram of the SIMRUN subroutine. This subroutine calls the SIM subroutine written by the user. In other words, for each combination of factor levels needed, this subroutine calls SIM and obtains responses for the number of repetitions desired by the user.

MEAN Subroutine. Figure 13 is the flow diagram for the MEAN subroutine. This subroutine calculates the mean of each row of a matrix. In particular, this subroutine calculates the mean of the repetition responses obtained for each row of

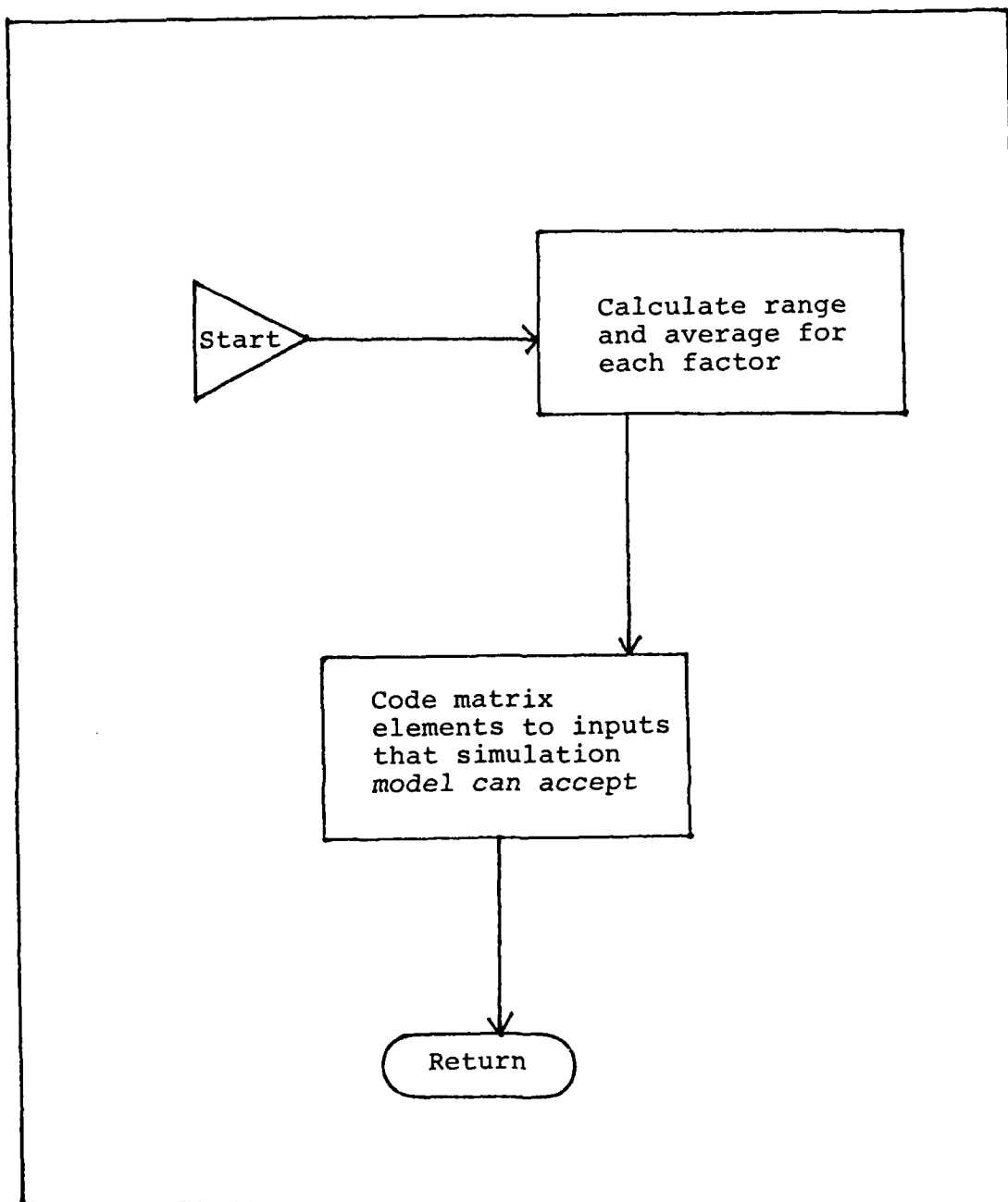


Figure 11. Flow Diagram of CODE Subroutine

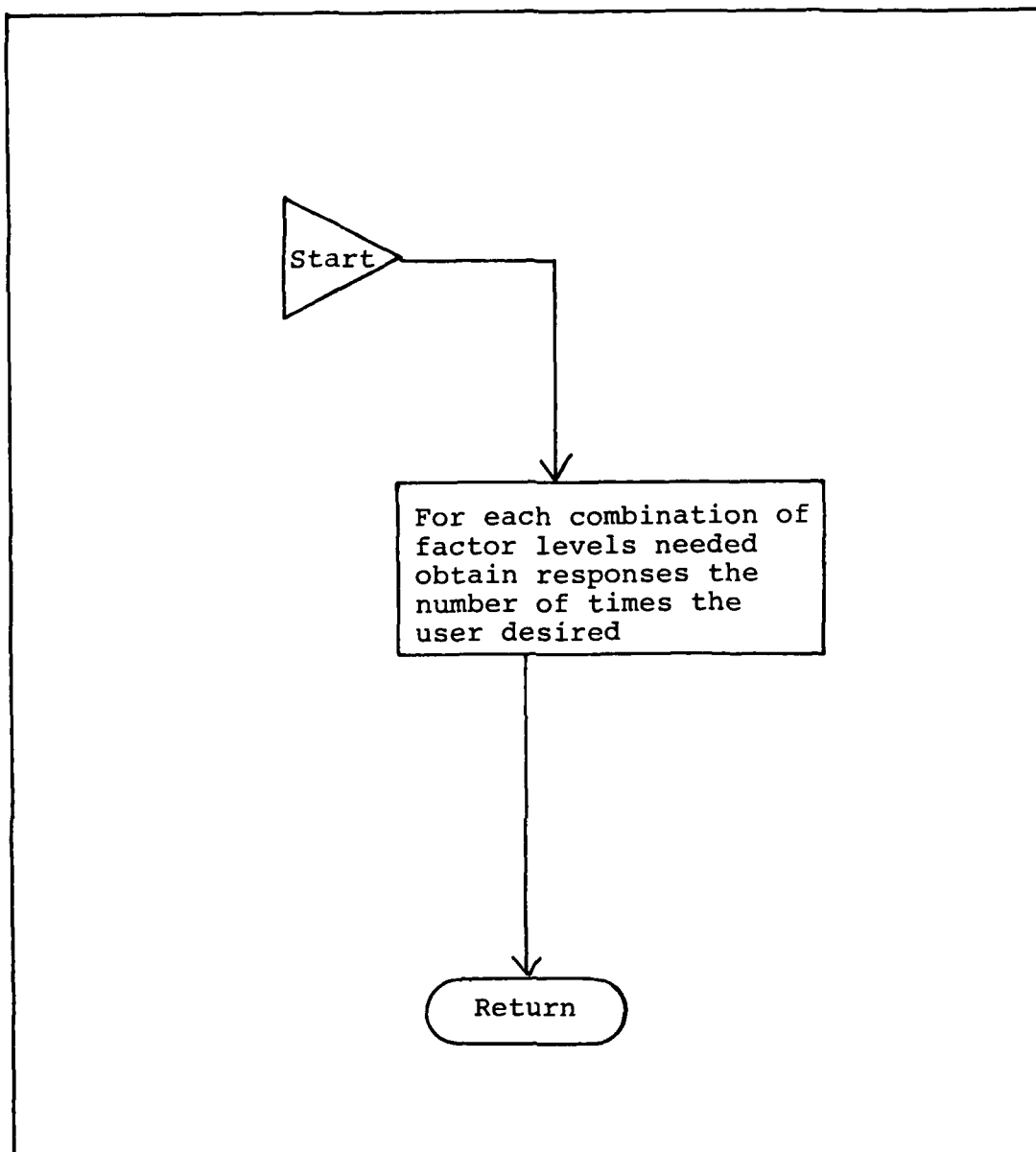


Figure 12. Flow Diagram of SIMRUN Subroutine



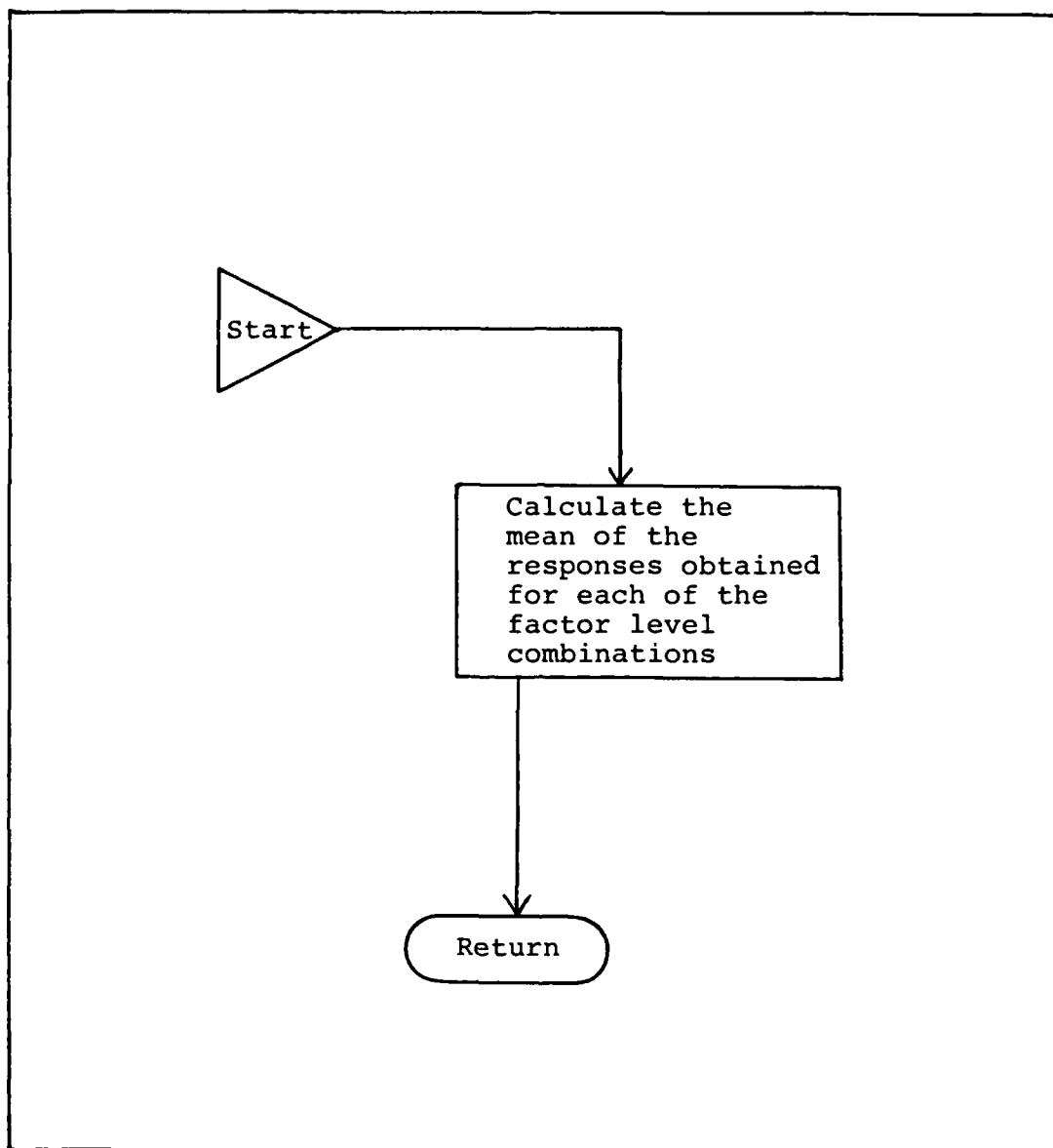


Figure 13. Flow Diagram of MEAN Subroutine

factor level combinations.

WRITE Subroutine. Figure 14 is the flow diagram for this subroutine. First, the file 'MATRIX' is opened, then the subroutine augments the design matrix on the right with the vector of average responses obtained. Next, the subroutine writes the design matrix, augmented with the average response vector, to the permanent file 'MATRIX' with proper format. This file, 'MATRIX', can now be used as data in a statistical package of the user's choice.

#### Regression Phase

This section will discuss the regression phase in six parts: (1) least squares procedure, (2) discussion of flow diagram, (3) determining lack-of-fit, (4) test statistic calculations, (5) regression output, and (6) verification of regression phase.

Least Squares Procedure. The classical method of fitting data is used in this program. This method was discussed in Chapter 2, Literature Review, and is called the method of least squares. Basically, the input needed is the design matrix, named  $X$  in this phase, and the vector of average responses obtained from running the simulation model, called  $Y$ . The estimated coefficients of the first-order and second-order models are found by the equation  $b = (X'X)^{-1}X'Y$ . To calculate the sum of squares due to the regression, the equation is  $SS_{reg} = b'X'Y$  and the total sum of squares equals  $SS_{tot} = Y'Y$ . These equations and other equations pertinent to

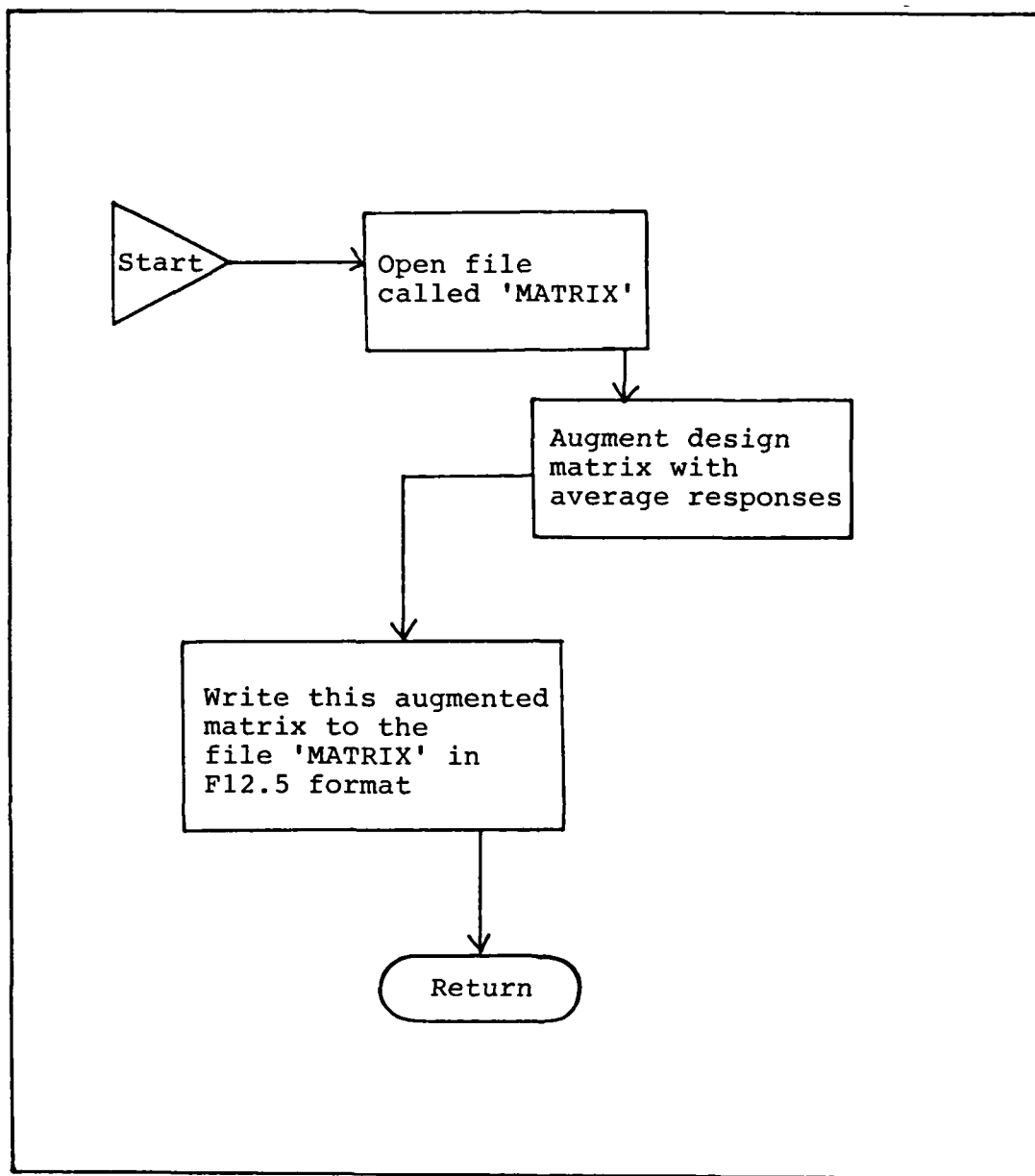


Figure 14. Flow Diagram of WRITE Subroutine

output statistics are discussed in the following sections.

Discussion of Flow Diagram. Figure 15 is the flow diagram of the REGRES subroutine. The first procedure is to calculate the degrees-of-freedom for normal least squares procedure -- total degrees-of-freedom, regression degrees-of-freedom, and residual degrees-of-freedom. The next five steps describe the calculations necessary to determine  $b$  from  $b = (X'X)^{-1}X'Y$ . All of the operations -- transpose, multiply, and inverse calculations are performed by calls to subroutines with appropriately passed arguments. The inverse subroutine was taken from Elementary Numerical Analysis: An Algorithmic Approach, published in 1980 (18).

The next three boxes generalize the operations to calculate the sum of squares due to regression. Following this, the subroutine calculates the sum of squares total uncorrected for the mean, and the difference between the total sum of squares and the regression sum of squares is the sum of squares due to the residual. The corresponding mean squares are then calculated by dividing each sum of squares by its applicable degrees-of-freedom. The next procedure is to calculate the estimated variances of the coefficients ( $\text{var}(b) = (X'X)^{-1}MS_{\text{res}}$ ) and their estimated standard errors ( $\text{s.e.}(b) = \sqrt{\text{var}(b)}$ ). After this, the  $t$ -statistics are calculated ( $t = b/\text{s.e.}(b)$ ). Next, the sum of squares total and sum of squares regression (corrected for the mean) are calculated. These will be used later to calculate the  $R$ -square value for the model, that is, the percentage of

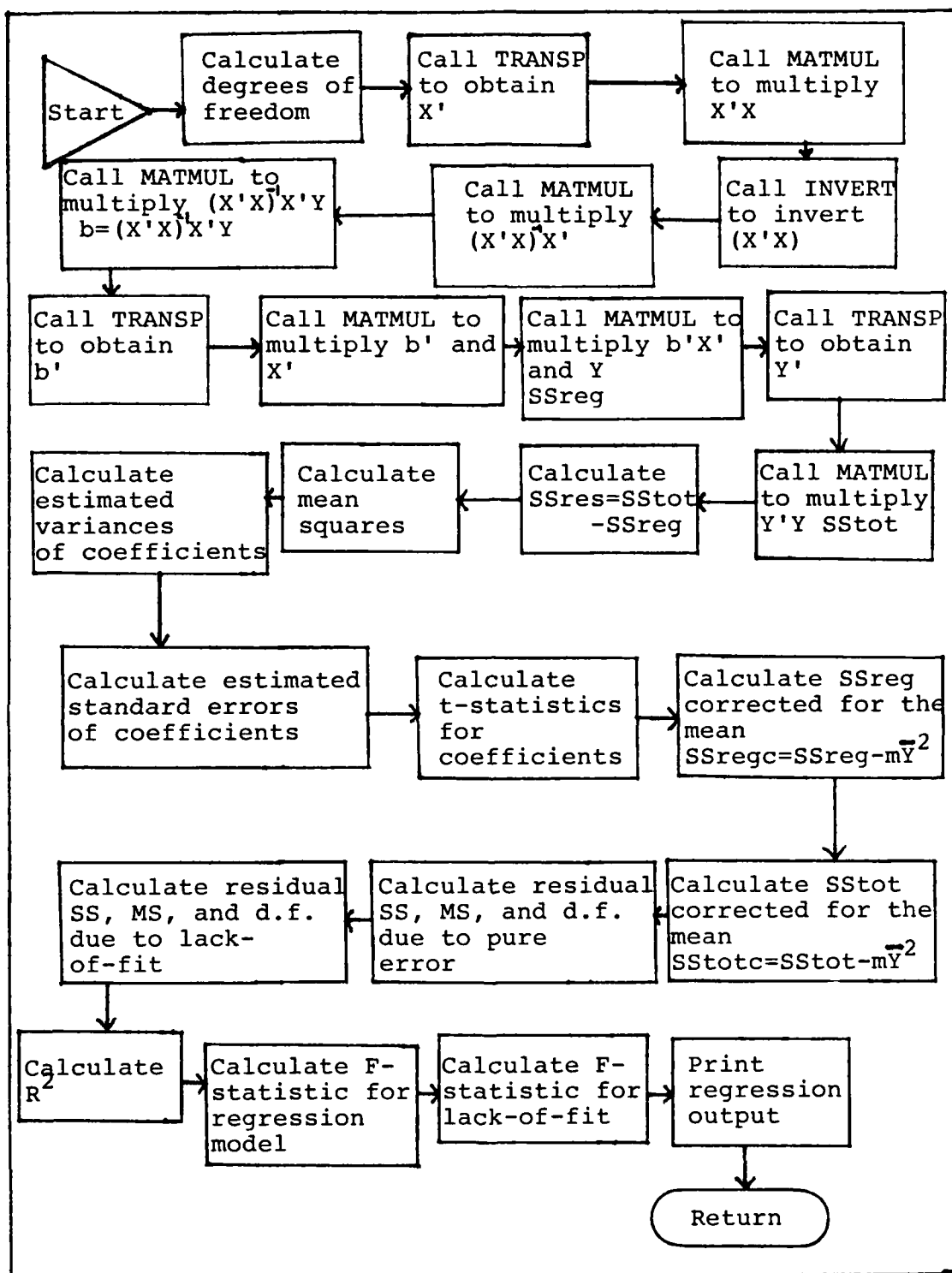


Figure 15. Flow Diagram of REGRES Subroutine

variation in the responses accounted for by the model.

The next two blocks describe the calculations needed to determine lack-of-fit statistics. These will be discussed in more detail in a following section. The last blocks show the calculation of statistics needed to allow the user to evaluate the estimated model adequacy. The following are questions to be answered. How well does the model explain the variation in the responses? Is the estimated model a 'good fit' of the model implicit in the simulation code? Are there higher order terms that should be included to depict the variable relationships embedded in the computer model? Following the calculation of the statistics needed to answer these questions, the regression subroutine ends by printing the regression output.

Determining Lack-of-Fit. Each of the generated designs has a certain number of center point rows. These center point rows, as mentioned previously, give an estimate of the pure error in the simulation model. Figure 16, taken from Applied Regression Analysis (21:29), depicts the breakup of residual sum of squares into its component parts, pure error sum of squares and lack-of-fit sum of squares. The pure error sum of squares calculated is the total sum of squares at the center points minus the correction factor for the mean at the center points ( $SS_{pe} = Y'Y - n_1\bar{Y}^2$ ), where  $n_1$  is the number of center points,  $\bar{Y}$  is the mean response of the center points, and  $Y$  are the responses obtained at the center point rows. The lack-of-fit sum of squares is obtained by

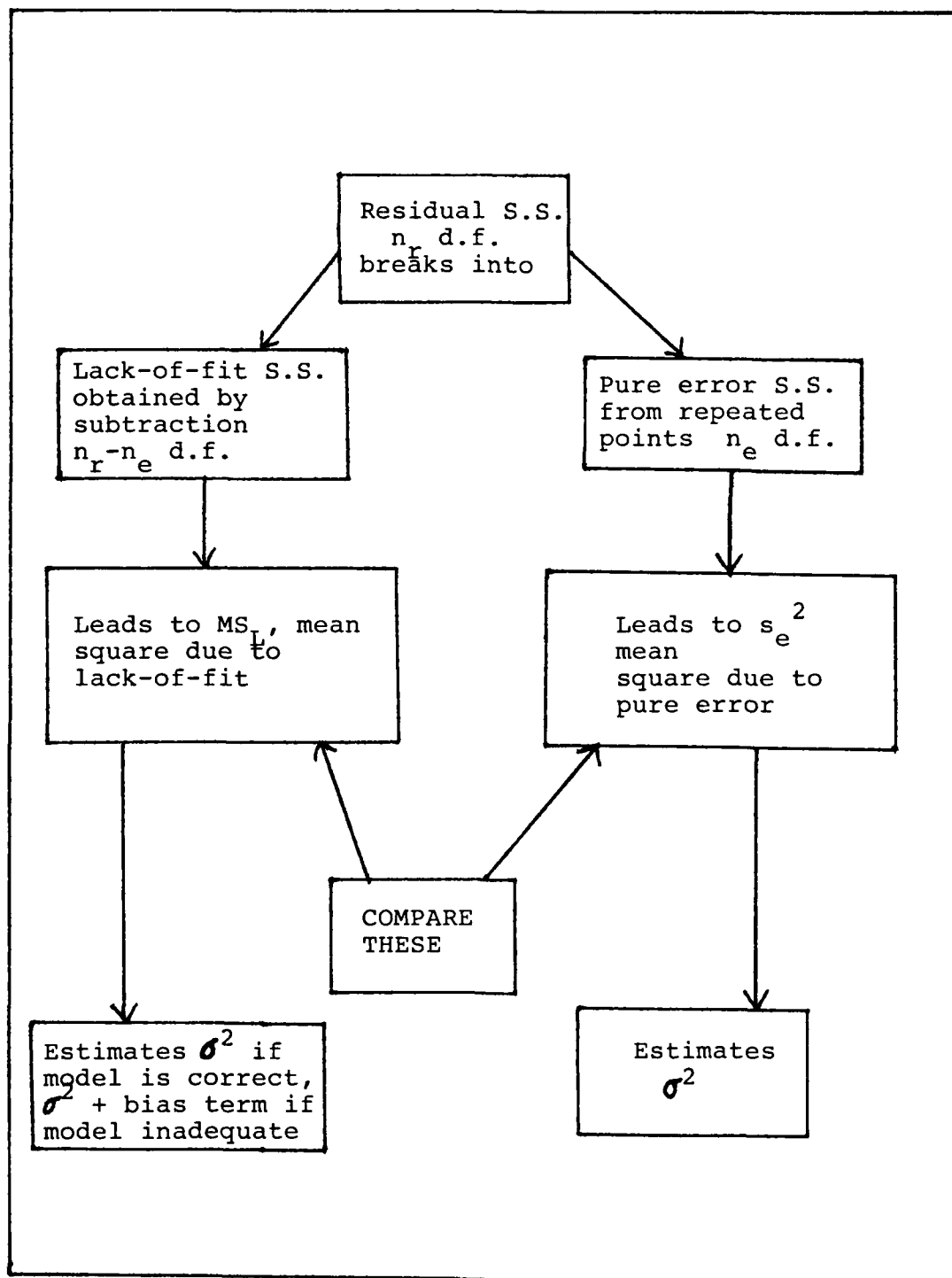


Figure 16. Breakdown of Residual Sum of Squares (21:29)

subtraction ( $SS_{lac} = SS_{res} - SS_{pe}$ ). The sum of squares due to pure error estimates  $\sigma^2$  and the sum of squares due to lack-of-fit estimates  $\sigma^2$  plus a bias term if higher order terms should have been included in the proposed model. The test statistic used to test for lack-of-fit is addressed in the next section.

Test Statistic Calculations. The test statistics provided by this program are t-statistics for each of the estimated coefficients, an F-statistic for the regression model, an F-statistic for lack-of-fit, and an Rsquare statistic. The t-statistics are calculated by  $t = b/s.e.(b)$ . Also listed are the degrees-of-freedom. With these two numbers, the user can look up the critical value in a t-table, and at a chosen  $\alpha$ -level, conclude whether or not each coefficient is significantly different from zero. The F-statistic for the regression model and the F-statistic for the lack-of-fit are calculated by these equations:  $F_{reg} = MS_{reg}/MS_{res}$ , and  $F_{lac} = MS_{lac}/MS_{pe}$ . They are also given with their associated degrees-of-freedom listed beside them. Again, this enables the user at a chosen  $\alpha$ -level to find the critical values and conclude whether the regression model proposed is significant and whether the lack-of-fit of the proposed model is significant. The Rsquare equals  $SS_{regc}/SS_{totc}$ . The interpretation is as discussed previously. Rsquare is the percentage of variation in the responses accounted for by the regression model proposed.

Regression Output. An example of some sample output is



given in Table VII included in the verification section which follows. Table VI shows how the output is listed and also includes the equations used for all the calculations. These equations will give the user further understanding of the least squares procedure used.

Regression Phase Verification. A significant amount of effort was involved in checking out this routine, since it used many other subroutines. As a result, a great deal of time was initially spent checking passed arguments and correct functioning of each subroutine called. Once all the subroutines called checked out, the verification process for this regression phase was essentially one of comparison. In the article by Cooley and Houck (19), they use a modified response surface methodology technique with a simulation model to determine the optimum response. They included in their article the design matrices and average responses obtained for first-order and second-order models. Their ANOVA table and estimated coefficients are slightly different, due to the fact that they subtracted out the block effect due to their variance reduction technique. Nevertheless, since their study and corresponding data were real, their data were used as a check-out for this routine. Table VII shows the design matrix used and the corresponding average responses obtained from their simulation runs. This data from their article were used as data for this regression routine, and also were used with the SPSS regression package. Table VIII is the output generated from the regression phase

TABLE VI  
Regression Output Equations

ANOVA for Response Surface Methodology			
Source	d.f.	SS	MS
Regression	n	b'X'Y	b'X'Y/n
Residual	m-n	Y'Y-b'X'Y	(Y'Y-b'X'Y) / (m-n)
Pure Error	nl-1	Y'Y-nl $\bar{Y}$ <sup>2</sup>	SSpe/(nl-1)
Lack of Fit	m-n-(nl-1)	difference	SSLac/(m-n-(nl-1))
Total	m	Y'Y	-----
F-statistic for Regression Model = $\frac{MS_{reg}}{MS_{res}} \approx F_{(n,m-n)}$			
F-statistic for Lack-of-Fit = $\frac{MS_{lac}}{MS_{pe}} \approx F_{(m-n-nl+1,nl-1)}$			
% Variance Explained = $R^2_{(corrected)} = \frac{SS_{regc}}{SS_{totc}}$			
Beta Estimates		standard error(b)	t-statistic
$b(0) = \frac{\sum y_i}{m}$			$\frac{b(0)}{s.e.(b(0))}$
$b(1) = \frac{\sum x_1 y_i}{\sum (x_1^2)}$		$V(b) = (X'X)^{-1}MS_{res}$	$\frac{b(1)}{s.e.(b(1))}$
⋮			⋮
$b(n) = \frac{\sum x_n y}{\sum (x_n^2)}$			$\frac{b(n)}{s.e.(b(n))}$
t-statistics $\approx T_{(m-n)}$			

TABLE VII

## Data Used for Regression Verification

<u>Design Matrix</u>	<u>Average Responses</u>
1 -1 -1	6276.72
1 -1 1	4853.87
1 1 -1	2661.70
1 1 1	3194.98
1 0 0	3760.15
1 0 0	3461.88
1 0 0	3343.83
1 0 0	3657.06

First-Order Data

<u>Design Matrix</u>	<u>Average Responses</u>
1 -1 -1 1 1 1	6276.72
1 -1 1 1 1 -1	4853.87
1 1 -1 1 1 -1	2661.70
1 1 1 1 1 1	3194.98
1 -1.414 0 2 0 0	6386.47
1 1.414 0 2 0 0	3112.45
1 0 -1.414 0 2 0	3174.38
1 0 1.414 0 2 0	3814.52
1 0 0 0 0 0	3760.15
1 0 0 0 0 0	3461.88
1 0 0 0 0 0	3343.83
1 0 0 0 0 0	3657.06
1 0 0 0 0 0	3608.6
1 0 0 0 0 0	3042.61

Second-Order Data

TABLE VIII  
First-Order Design Output

ANOVA for Response Surface Methodology

SOURCE	d.f.	SS	MS
Regression	3	128910880.000000	42970292.000000
Residual	5	2017568.000000	403513.593750
Pure Error	3	105760.000000	35253.332031
Lack of Fit	2	1911808.000000	955904.000000

Total 8 130928448.000000

F-statistic for Regression Model= .106490318e+03 d.f.= 3 , 5

F-statistic for Lack of Fit= .271152802e+02 d.f.= 2 , 3

Rsquare (corrected for mean) = .779955983e+00

degrees of freedom for t-statistics= 5

Beta Estimates standard error(b) t-statistic

b( 0)= 3901.27417 224.58673 17.37090  
b( 1)= -1318.47766 317.61359 -4.15120  
b( 2)= -222.39252 317.61359 -.70020

of this program and Table IX the output generated from the SPSS regression package for the first-order model given by  $Y=B_0+B_1X_1+B_2X_2$ . The estimated coefficients are the same, and their associated standard errors are also the same. Since the t-statistic is the square root of the F-statistic, the statistics given for the estimated coefficients all check. The residual sum of squares and mean square checks out with the SPSS output. In SPSS, the regression sum of squares is given corrected for the mean. The correction factor is  $m\bar{Y}^2=8 \times (3901.274)^2$  and the difference between SSreg in this package and  $m\bar{Y}^2$  is SSreg in the SPSS printout. The F-statistic for the regression model in this package was the same as given in the SPSS package. The Rsquare value checked as well. All calculations checked out with a first order model. This same comparison procedure was used with the central composite design and corresponding average responses from the same article to check this routine with a second-order model. The output from this regression routine and the SPSS check are given in Table X. Again, all the calculations in this routine checked.

#### Subsequent Subroutines

Following the regression phase, the only processes left undone are the uncoding (flow diagram shown in Figure 17) of the estimated coefficients and the copying of the generated design matrix and corresponding average responses to other storage locations to be accessible for comparison purposes,

TABLE IX

## SPSS First-Order Design Output

MULTIPLE R	.8832	ANOVA	DF	SUM SQUARES	MEAN SQ.	F
R SQUARE	.7800	REGRESSION	2.	7151365.368	.358E+07	8.861
STD DEV	635.2291	RESIDUAL	5.	2017579.747	.404E+06	SIG. .023
ADJ R SQUARE	.6919	COEFF OF VARIABILITY		16.3PCT		
VARIABLE	B	S.E. B	F	SIG.	BETA	ELASTICITY
X1	-1318.477	317.615	17.232	.009	-.87085	0
X2	-222.392	317.615	.490	.515	-.14689	0
CONSTANT	3901.274	224.587	301.746	.000		

TABLE X  
Second-Order Design Output  
ANOVA for Response Surface Methodology

SOURCE	d.f.	SS	MS
Regression	6	227487600.000000	37914600.000000
Residual	8	822048.000000	102756.000000
Pure Error	5	336560.000000	67312.000000
Lack'of Fit	3	485488.000000	161829.328125

Total 14 228309648.000000

F-statistic for Regression Model= .368976990e+03 d.f.= 6 , 8

F-statistic for Lack of Fit= 2.40416765 d.f.= 3 , 5

Rsquare (corrected for mean) = .952540576e+00

degrees of freedom for t-statistics= 8

Beta Estimates standard error(b) t-statistic

b( 0)=	3479.02539	130.86635	26.58457
b( 1)=	-1238.10889	113.34213	-10.92364
b( 2)=	1.94879	113.34213	.01719
b( 3)=	666.43396	117.96133	5.64960
b( 4)=	38.92819	117.96133	.33001
b( 5)=	489.03253	160.27788	3.05115

TABLE X

## Second-Order Design Output

MULTIPLE R		.9760 ANOVA		DF	SUM SQUARES	MEAN SQ.	F
R SQUARE		.9525 REGRESSION		5.	.165E+08	.330E+07	32.115
STD DEV		320.5466 RESIDUAL		8.	822001.085	.103E+06	SIG. .000
ADJ R SQUARE		.9229 COEFF OF VARIABILITY		8.3PCT			
VARIABLE	B	S.E. B	F	SIG.	BETA	ELASTICITY	
X1	-1238.109	113.339	119.333	.000	-.84136	0	
X2	1.949	113.339	.000	.987	.00132	0	
X1SQ	666.592	117.984	31.921	.000	.43644	.09810	
X1X2	489.033	160.273	9.310	.016	.23501	0	
X2SQ	38.898	117.984	.109	.750	.02547	.00572	
CONSTANT	3479.012	130.863	706.774	.000			

SPSS Output



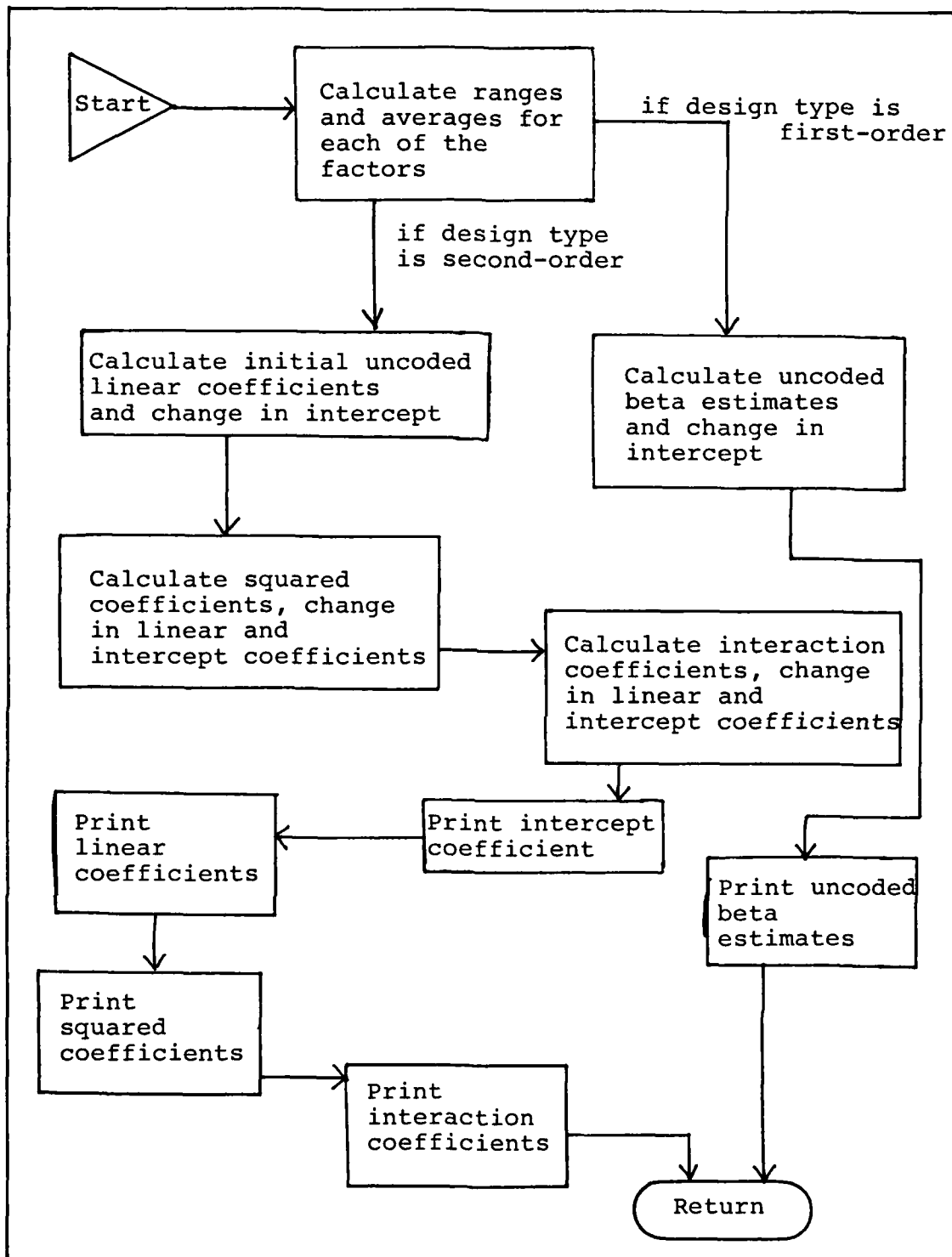


Figure 17. Flow Diagram of UNCODE Subroutine

if needed.

The reason for the UNCODE subroutine is basically the problem that the estimated coefficients from the regression routine are in terms of the design matrix. For example, a one in the design matrix stands for

$$1 = (\text{high}(\text{factor}) - \text{ave}(\text{factor})) / \text{range}(\text{factor}) / 2).$$

The estimated coefficients need to be translated into coefficients that reflect the proper ranges of the input factors. For example, refer to the data used to obtain the regression output in Table X. Factor 1 had high and low values of 100 and 50, respectively. 240 and 160 were the high and low values of factor 2. Therefore, the ranges and averages of the factors were:

$$\begin{aligned} \text{ave}(X_1) &= 75 & \text{ave}(X_2) &= 200 \\ \text{range}(X_1) &= 50 & \text{range}(X_2) &= 80 \\ \text{range}(X_1)/2 &= 25 & \text{range}(X_2)/2 &= 40 \end{aligned}$$

In the design matrix the coding was as follows:

$$\begin{aligned} \text{for } X_1: \quad 1 &= (100 - 75) / 25 \\ \quad 0 &= (75 - 75) / 25 \\ \quad -1 &= (50 - 75) / 25 \\ \text{for } X_2: \quad 1 &= (240 - 200) / 40 \\ \quad 0 &= (200 - 200) / 40 \\ \quad -1 &= (160 - 200) / 40 \end{aligned}$$

The estimated regression equation in terms of the design matrix was:

$$\begin{aligned} \hat{Y} = & 3479.02539 - 1238.10889X_1 + 1.94879X_2 + 666.43396X_1^2 \\ & + 38.92819X_2^2 + 489.03253X_1X_2. \end{aligned}$$

This equation needs to be uncoded to be in terms of the original factors. The algorithm which accomplishes this is as follows:

$$\begin{aligned} \hat{Y}_m = & 3479.02539 - 1238.10889 \left( \frac{X_1 - 75}{25} \right) + 1.94879 \left( \frac{X_2 - 200}{40} \right) \\ & + 666.43396 \left( \frac{X_1 - 75}{25} \right)^2 + 38.92819 \left( \frac{X_2 - 200}{40} \right)^2 \\ & + 489.03253 \left( \frac{X_1 - 75}{25} \right) \left( \frac{X_2 - 200}{40} \right) . \end{aligned}$$

The UNCODE subroutine which calculates the new estimated coefficients in terms of the original factors was checked out by hand and printed traces. Table XI shows the uncoded estimates for both the first-order model and the second-order model obtained in Tables VIII, IX, and X.

The COPY subroutine performs one function -- copies any matrix 'A' to a matrix 'B'. This subroutine is called twice at the end of the main program. The first time is to copy the design matrix 'A' to matrix 'AA'. Next, it is called to copy the matrix of average responses 'YAVE' to matrix 'YYAVE'. Both of these copied matrices are used in the subroutine COMPAR, if the program is sequentially run.

#### Verification of Entire Program

The program verification was performed in stages. As discussed previously, each main section was checked individually. The design generation phase was the first section of the program written. It was checked out following its completion by the methods discussed in the design verification phase section. Likewise, the regression phase

TABLE XI  
Uncoded Coefficients

Uncoded Beta Estimates

-----  
b( 0)= 8968.66992  
b( 1)= -52.73911  
b( 2)= -5.55981  
-----

First-Order

Uncoded Beta Estimates

-----  
b(0)= .214902070e+05  
b(1)= -307.2750244  
b(2)= -46.3607712  
b(1,1)= 1.0662943  
b(2,2)= .0243301  
b(1,2)= .4890325  
-----

Second-Order

was verified as discussed earlier. To verify the entire program flow certain processes during execution needed to be checked. Was the design type requested generated correctly? Was the generated design matrix coded to inputs that the simulation model could accept? Were the average responses for each combination of factor levels needed obtained? Was the permanent file 'MATRIX' written and does it contain all the correct information? If the regression portion was desired did the REGRES subroutine perform all the operations correctly? A method was needed to check all these processes simultaneously. The Cooley and Houck article (19) contained the data as they proceeded through their response surface experimentation. For their first-order model they used the full  $2^k$  design with four added center points. The number of factors was two so that the total number of rows in the design for the first-order phase was eight. They listed their high and low values for each factor. They are as follows:

	high	low
factor $X_1$ :	100	50
factor $X_2$ :	240	160.

These high and low levels given for each factor defined the coded design matrix that would be input into their simulation model. They listed this coded design matrix as well as the obtained average responses from their simulation model runs. These data were used to check the RSM program for a first-order model. The subroutine SIM listed in Figure 18

```

      subroutine sim(c,y1,j,k)
* This subroutine is for a check with dummy data

      integer j,k
      real c(300,300),y1,t

      t=.1

      if (c(j,1) .eq. 50. .and. c(j,2) .eq. 160.) then
        y1=6276.72
      else if (c(j,1) .eq. 50. .and. c(j,2) .eq. 240.) then
        y1=4853.87
      else if (c(j,1) .eq. 100. .and. c(j,2) .eq. 160.) then
        y1=2661.70
      else if (c(j,1) .eq. 100. .and. c(j,2) .eq. 240.) then
        y1=3194.98
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3760.15
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3461.88
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3343.83
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3657.06
      else if (c(j,1) .eq. 39.65 .and. c(j,2) .eq. 200.) then
        y1=6386.47
      else if (c(j,1) .eq. 110.35 .and. c(j,2) .eq. 200.) then
        y1=3112.45
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 143.44) then
        y1=3174.38
      else if (c(8,1) .eq. 75. .and. c(j,2) .eq. 256.56) then
        y1=3814.52
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3608.62
      else if (c(j,1) .eq. 75. .and. c(j,2) .eq. 200.) then
        y1=3042.61
      else
        print *, 'sim not working correctly'
      endif

      end

```

Figure 18. Subroutine SIM for Check

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AN INTERACTIVE COMPUTER PACKAGE FOR USE WITH SIMULATION 2/3

MODELS WHICH PERF. (U) AIR FORCE INST OF TECH

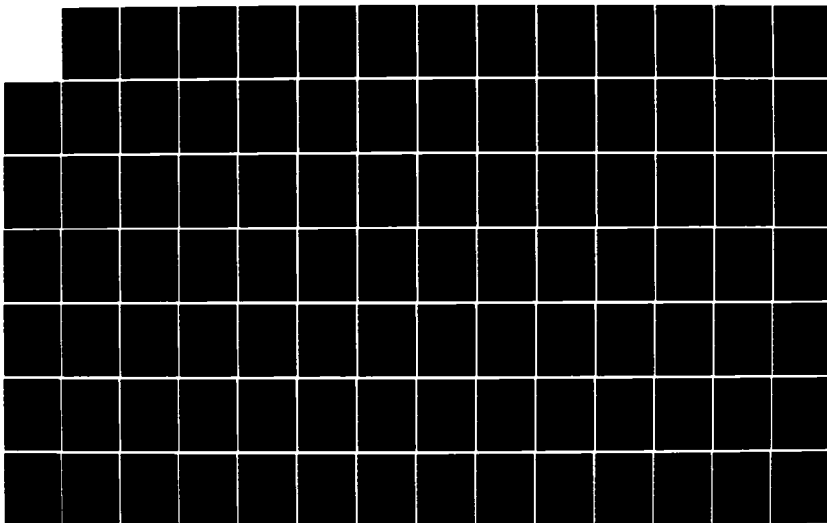
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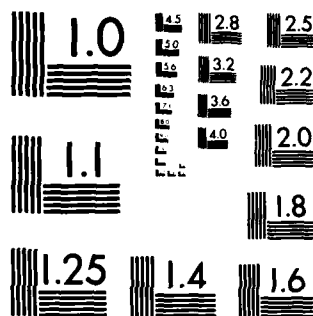
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gives the average response that would have been obtained from their simulation model if a particular combination of factor levels was used as input. If, when this RSM program is run, correct average responses are obtained for particular combinations of factor levels then this program is generating the correct design matrix and the corresponding correct coded design matrix. Correct average responses were obtained and the generated designs during the intermediate processes were printed for debugging purposes. Table XII is the data that were generated during execution of the RSM program. These data all checked with the data from the Cooley and Houck article. A second-order model check was performed in the same manner. Again they were testing two input factors; but, the central composite design they used during experimentation contained six center points, whereas, the central composite design for two factors offered by the RSM program uses nine center points. Because of this discrepancy, the user input design subroutine was used to input the needed design matrix. Table XIII lists the data generated during the execution of the RSM program. All these generated data from the RSM program checked with the data used in the Cooley and Houck study. From this set of checks the internal processes of the program were verified.

#### Program Limitations

Inherent in any research effort are limitations. The limitations present during this research covered three areas:

TABLE XII  
First-Order Model Check

<u>Design Matrix</u>	<u>Simulation Matrix</u>		<u>Average Responses</u>
1 -1 -1	50	160	6276.72
1 -1 1	50	240	4853.87
1 1 -1	100	160	2661.70
1 1 1	100	240	3194.98
1 0 0	75	200	3760.15
1 0 0	75	200	3461.88
1 0 0	75	200	3343.83
1 0 0	75	200	3657.06

File 'MATRIX'

1.00000	-1.00000	-1.00000	6276.72021
1.00000	-1.00000	1.00000	4853.87012
1.00000	1.00000	-1.00000	2661.69995
1.00000	1.00000	1.00000	3194.97998
1.00000	.00000	.00000	3760.14990
1.00000	.00000	.00000	3461.87988
1.00000	.00000	.00000	3343.83008
1.00000	.00000	.00000	3657.06006

TABLE XIII  
Second-Order Model Check

Design Matrix						Simulation Matrix		Average Responses
1	-1.000	-1.000	1	1	1	50	160	6276.72
1	-1.000	1.000	1	1	-1	50	240	4853.87
1	1.000	-1.000	1	1	-1	100	160	2661.70
1	1.000	1.000	1	1	1	100	240	3194.98
1	-1.414	.000	2	0	0	39.65	200	6386.47
1	1.414	.000	2	0	0	110.65	200	3112.45
1	.000	-1.414	0	2	0	75	143.44	3174.38
1	.000	1.414	0	2	0	75	256.56	3814.52
1	.000	.000	0	0	0	75	200	3760.15
1	.000	.000	0	0	0	75	200	3461.88
1	.000	.000	0	0	0	75	200	3343.83
1	.000	.000	0	0	0	75	200	3657.06
1	.000	.000	0	0	0	75	200	3608.62
1	.000	.000	0	0	0	75	200	3042.61

File 'MATRIX'				
1.00000	-1.00000	-1.00000	1.00000	1.00000
1.00000	6276.72021			
1.00000	-1.00000	-1.00000	1.00000	1.00000
-1.00000	4853.87012			
1.00000	1.00000	-1.00000	1.00000	1.00000
-1.00000	2661.69995			
1.00000	1.00000	1.00000	1.00000	1.00000
1.00000	3194.97998			
1.00000	-1.41400	.00000	2.00000	.00000
.00000	6386.47021			
1.00000	1.41400	.00000	2.00000	.00000
.00000	3112.44995			
1.00000	.00000	-1.41400	.00000	2.00000
.00000	3174.37988			
1.00000	.00000	1.41400	.00000	2.00000
.00000	3814.52002			
1.00000	.00000	.00000	.00000	.00000
.00000	3760.14990			
1.00000	.00000	.00000	.00000	.00000
.00000	3461.87988			
1.00000	.00000	.00000	.00000	.00000
.00000	3343.83008			
1.00000	.00000	.00000	.00000	.00000
.00000	3657.06006			
1.00000	.00000	.00000	.00000	.00000
.00000	3608.62012			
1.00000	.00000	.00000	.00000	.00000
.00000	3042.61011			

computer system limitations, time constraints, and limitations of computer code.

The limitations of any computer system on which this program is used deal with the amount of core allowed to run a single program and the inability of the system to restart jobs following system downtimes. The Vax 11/780 does not allow enough core to run this program with the matrices declared large enough for 512 rows (needed to run the full  $2^9$ ). This allotted core space will differ from system to system, and matrix dimensions will have to be changed accordingly. Also, if the system goes down while the program is running, it cannot be started where it left off. The program must be run from start to finish to retain the information needed to produce the program output. From system to system the methods for opening and closing permanent files will differ, and the open statements present in this program will need to be changed.

Several enhancements could be added to this program to make it more useful and flexible, but could not be added during this research effort due to lack of time. An optimization phase could be added after the regression phase to locate the maximum or minimum of the estimated response surface. If the optimum occurred at a boundary of the input experimental region, the user could sequentially shift the experimental region without having to stop and restart the program each time. Also, at this time, the program only handles two to nine factors. The limit on the number of

factors allowed could be increased as an enhancement. A further enhancement might be to offer a set of designs capable of accounting for a block effect. Adding this type of provision would require revision of the design generation phase and the regression phase.

Other limitations deal with creating unlimited numbers of files and storage locations during program execution. At this time, during the COPY subroutine, the design matrix 'A' is always copied to 'AA' and the average responses, 'YAVE', are always copied to 'YYAVE'. This means that 'AA' and 'YYAVE' always contain the most recently used design matrix and obtained average responses. Thus, in the COMPARE subroutine, the comparison is only between the generated design matrix for this present run and the generated design matrix for the most recently completed run. Similar to this file problem is the creation of the permanent file 'MATRIX'. Every time the program is executed, the generated design matrix, augmented with the corresponding average responses obtained, is written to the file 'MATRIX' to be used if desired. Each time this program is run, the file 'MATRIX' is overwritten. Even though limitations exist inherently in this program, the benefits of program usage far outweigh the limits. The next chapter describes the application of this RSM program to a simulation model.

## V. Application of RSM Program

This chapter discusses the actual application of the response surface methodology program to a simulation model. This application is discussed in four sections: (1) Description of Simulation Model, (2) Analysis Objectives, (3) Problem Setup, and (4) Program Output.

### Description of Simulation Model

The simulation model chosen was a combined SLAM (Simulation Language for Alternative Modeling) network-FORTRAN discrete event model. This simulation model was developed by Joseph Bryant and Stephen Gordon as their thesis effort. (15) The purpose of their study was to develop a cargo aircraft scheduling model that incorporated user needs to evaluate the end user satisfaction. They developed, by a modified worth assessment technique, estimates of the relative worth of each supply category. Table XIV depicts the general worths for each supply class generated by the modified worth assessment procedure used.

To measure overall airlift score, they calculated a score for each simulation run. This overall score was basically calculated as

$$\text{Score} = \sum_{i=\text{class I}}^{\text{class IX}} ((\text{actual}_i / \text{desired}_i) \times W_i) .$$

A simplified definition is: for each supply class the actual level delivered was divided by the desired level and

TABLE XIV  
Supply Class Worths

<u>Class</u>	<u>Description</u>	<u>Worth Value</u>
IX	Repair Parts and Components	12.8
III	POL	12.7
V	Ammunition	11.0
VIII	Medical Supplies	9.0
I	Subsistence	7.0
IV	Construction Materials	4.0
II	Clothing and Equipment	1.0
VI	Personal Demand Items	0.5
VII	Major End Items	1.0

multiplied by the assessed worth. The score for each supply class is then combined into an overall supply score.

The input for the simulation model is a multiplier set for the supply classes. This multiplier set adjusts each initial unweighted priority. The resulting weighted priority is entered into the scheduling process. Intuitively, if the worth values are input as the multiplier set, the overall score should be a maximum. This does not occur. Because of the queueing buildups, when the multipliers are input as their assessed worth values, the score is suboptimal.

#### Analysis Objectives

As a result of this queueing buildup, it is desirable to find out how the response surface is responding to differing supply class priorities. The factors which have the most impact on the output score are Repair Parts and Components, POL, and Ammunition. Therefore, these three factors were chosen to use as input factors in the RSM program. The remaining input factors to the simulation model were set at their assessed worth value. The objective was to explore the response surface in an experimental region defined by the assessed worth values of the three input factors. Table XV shows the experimental region chosen. Information about the curvature of the response surface was desired; therefore, a second-order design was needed. The second-order design chosen was the central composite design. Table XVI lists the central composite design for three factors. The estimated



TABLE XV  
Experimental Region for Simulation Runs

	<u>Description</u>	<u>Worth Value</u>	<u>High Level</u>	<u>Low Level</u>
IX	Repair Parts and Components	12.8	15.6	10.0
III	POL	12.7	15.4	10.0
V	Ammunition	11.0	13.0	9.0

TABLE XVI

## Three Factor Central Composite Design

1.0	-1.0	-1.0	-1.0	1.0	1.0	1.0	1.0	1.0	1.0
1.0	-1.0	-1.0	1.0	1.0	1.0	1.0	1.0	-1.0	-1.0
1.0	-1.0	1.0	-1.0	1.0	1.0	1.0	-1.0	1.0	-1.0
1.0	-1.0	1.0	1.0	1.0	1.0	1.0	-1.0	-1.0	1.0
1.0	1.0	-1.0	-1.0	1.0	1.0	1.0	-1.0	-1.0	1.0
1.0	1.0	-1.0	1.0	1.0	1.0	1.0	-1.0	1.0	-1.0
1.0	1.0	1.0	-1.0	1.0	1.0	1.0	1.0	-1.0	-1.0
1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1.0	-1.682	0.0	0.0	2.828	0.0	0.0	0.0	0.0	0.0
1.0	1.682	0.0	0.0	2.828	0.0	0.0	0.0	0.0	0.0
1.0	0.0	-1.682	0.0	0.0	2.828	0.0	0.0	0.0	0.0
1.0	0.0	1.682	0.0	0.0	2.828	0.0	0.0	0.0	0.0
1.0	0.0	0.0	-1.682	0.0	0.0	2.828	0.0	0.0	0.0
1.0	0.0	0.0	1.682	0.0	0.0	2.828	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

second-order model obtained from the RSM program will illuminate how each of these factors impacts the score. Furthermore, this estimated response surface can be searched to locate the optimum which previously had been embedded in the code of the simulation model.

#### Problem Setup

Because this simulation model was a combined SLAM network-FORTRAN discrete event model, a lot more changes and additions were required for program interface.

In a combined SLAM network-FORTRAN discrete event simulation model, all FORTRAN variables needing to be passed are passed by means of COMMON statements. In a FORTRAN program, those global variables included in COMMON statements cannot be passed by subroutine arguments. These requirements meant that in all FORTRAN subroutines that needed these variable values, COMMON statements had to be added and subroutine dummy arguments containing these variables had to be changed. For the COMMON variables, declaration statements had to be added and changed to insure that variable type was consistent throughout the program. Six subroutines and the main program required these revisions.

The program MAIN of the simulation model's FORTRAN discrete event section had to be renamed subroutine SIM. Every time a response was needed, the Response Surface Methodology Program would call the subroutine SIM which, in turn, would call SLAM. This statement (call SLAM) would

execute the combined SLAM network-FORTRAN discrete event simulation model.

The subroutine INTLC contained in the FORTRAN discrete event section of the simulation model is the first subroutine called by the SLAM network. This subroutine is used to initialize the variables needed for the simulation model. Therefore, this subroutine needed to contain the assignment statements which input the values for the multiplier set to be used in the simulation runs. These assignments were accomplished by the following statements:

```
XX(71) = 7.0
XX(72) = 1.0
XX(73) = c(j,1)
XX(74) = 4.0
XX(75) = c(j,2)
XX(76) = 0.5
XX(77) = 1.0
XX(78) = 9.0
XX(79) = c(j,3)
```

where XX(71),...,XX(79) stand for the multiplier set input for supply classes I,...,IX; and, c(j,1), c(j,2), and c(j,3) are the input levels for supply classes III, V, and IX depending on the row of the input matrix for the simulation run. Note that the supply classes not chosen as input factors in the RSM program are set at their fixed assessed worth values.

The subroutine OTPUT in the FORTRAN discrete event section of the simulation model is the subroutine that formats and prints the output. In this subroutine an assignment needs to be made between the simulation model output variable and the response value that will be

transferred back to the RSM program. The assignment statement is:

```
nn = nn+1  
yy(nn) = value
```

where value is the simulation model output of the score achieved from the simulation run and yy(nn) is the response value to be transferred back to the RSM program.

The FORTRAN discrete event portion of the simulation model used unit numbers for output files, temporary files, and input files. Some of the unit numbers were the same for the RSM program. The unit numbers in the RSM program were changed so that no unit numbers were the same throughout the FORTRAN code.

Another needed change was a result of the implicit FORTRAN subroutines offered by the SLAM processor. The SLAM processor offers a FORTRAN subroutine named COPY. The RSM program also contained a subroutine named COPY. To take care of this name duplication, the subroutine COPY in the RSM program was renamed MCOPY.

Following all these needed changes and additions the RSM program and the FORTRAN discrete event portion of the simulation model were merged into one file. In order to run a SLAM simulation model, the FORTRAN part must already be compiled. The command to run this combined SLAM network-FORTRAN discrete event simulation model on the Vax 11/780 is:

```
slamlc -m ftn.o -i s2
```

where ftn.o is the compiled FORTRAN part and s2 is the SLAM

network. This command tells the SLAM processor to go to the FORTRAN MAIN program to begin execution and use the file s2 as the SLAM network input when the statement call SLAM is used. After the SLAM network is completed, the SLAM processor always returns to the FORTRAN MAIN program for further instructions. This automatic MAIN program return caused problems with the RSM program. Normally when a subroutine is called in FORTRAN after subroutine execution is completed, program execution continues immediately following the call statement to that subroutine. The SLAM processor overrides this normal FORTRAN flow. A series of IF statements had to be inserted in the RSM MAIN program to insure that program execution continued in the correct place.

The main problem with running this combined SLAM network- FORTRAN discrete event simulation model is that the SLAM network could not be called more than once during program execution. This means that even though the assignment of simulation output and response value was performed correctly, no more than one combination of factor levels could be obtained from a simulation model run. Because all the responses corresponding to the combinations of factor levels could not be obtained during RSM program execution, the complete response matrix is never assigned in the RSM program. Even though the RSM program could never complete execution because of the inherent limitations of the SLAM processor, the next section shows the RSM program processes were interfacing correctly with the simulation

model.

### Program Output

The SLAMOUT file generated by executing a SLAM file shows that the interface between the RSM program and the simulation model was performed correctly. The print statements included in the RSM program are included within the generated SLAMOUT file.

The FORTRAN MAIN program echoes the inputs desired by the user before continuing the RSM program execution. The inputs listed in the SLAMOUT file matched the inputs read into the RSM MAIN program. The echo was:

```
      You input k = 3  
      Design type = 4  
      Repetitions per run = 2.
```

The number of factors to be used was three, the design type to be used was the central composite design (design type four), and the number of repetitions per run requested was two.

The SLAM network was called correctly because the SLAMOUT file echoed the SLAM network requested as input and the normal SLAM output file is listed. Following the automatic SLAM output is the output generated by the ODPUT subroutine in the FORTRAN discrete event section of the simulation model.

Print statements were added to the FORTRAN discrete event section of the simulation model to verify that the COMMON variables were assigned correctly. COMMON variables

checked were the input levels for the three variables, the row number of the design matrix that was being used, and the output obtained for a simulation run to be returned as the response to the RSM program. Table XVII lists the matrix of factor level combinations to be used as input in the simulation model. Each time the SLAM network is initiated, a different row would be used as the factor inputs. The first column stands for the input level of class III, the second column is the input level of class V, and the third column is the input level of class IX. These input levels were verified by print statements which were output in the SLAMOUT file. The row to be used was listed and each of the factor levels assigned was listed prior to each simulation run.

The output obtained to be returned to the RSM program was verified also by a print statement listed in the SLAMOUT file.

When sequential runs of the SLAM network could not be obtained, the RSM program tried to continue its execution. The file 'MATRIX' written in the subroutine WRITE verified that the central composite design requested was generated correctly. The file 'MATRIX' also showed that responses for each factor level combination were not obtained because the SLAM network could not be called more than once. When execution proceeded to the subroutine REGRES which performs the regression, the RSM program cannot continue because the response vector contains all zeros. The program stops execution after trying to divide by zero.



TABLE XVII

## Matrix of Factor Level Combinations

<u>III</u>	<u>V</u>	<u>IX</u>
10.0	9.0	10.0
10.0	9.0	15.6
10.0	13.0	10.0
10.0	13.0	15.6
15.4	9.0	10.0
15.4	9.0	15.6
15.4	13.0	10.0
15.4	13.0	15.6
8.1586	11.0	12.8
17.2414	11.0	12.8
12.7	7.636	12.8
12.7	14.364	12.8
12.7	11.0	8.0904
12.7	11.0	17.5096
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8
12.7	11.0	12.8

Even though the RSM program never achieves completion, the outputs listed in the SLAMOUT file generated by the SLAM processor demonstrate that the Response Surface Methodology Program is interfacing correctly with the combined SLAM network-FORTRAN discrete event simulation model.

## VI. Conclusions and Recommendations

The overall objective of this research effort was to develop an interactive, user-friendly response surface methodology computer package which can be attached to any FORTRAN-based simulation model to yield a response function which describes the relationships between the input parameters and the output parameter of interest.

Subobjectives were:

- (1) After the response surface is generated, search this surface for the combinations of pertinent input parameters that yield the optimum response,
- (2) Interpret how the response function reveals the sensitivity of the output parameters due to changes in input parameters, and
- (3) Illustrate how the response function describes the relative ranking of effects on response between input parameters.

This research effort accomplished the overall objective and touched on subobjectives two and three.

The overall objective was accomplished by developing the RSM computer program. The user-friendly requirement meant the program had to be flexible and easy to understand. The input requirements were designed to be easily understood and proceed in a logical sequence. Five design types are offered by this program and also a user design input subroutine offers further flexibility. The user can use the regression

portion offered by this program or can choose to use the permanent file 'MATRIX', which is generated containing necessary data, to perform his/her own statistical analysis. The RSM program's modular design enables enhancements to be made with few changes to the program itself.

Subobjectives two and three were implicitly accomplished by the output displayed from the regression portion. The estimated coefficients and associated statistics illuminate the relationships between the input factors and reveal sensitivities in the response due to changes in input factors.

Much more time and research would have been required to accomplish subobjective one, the addition of a search phase to the RSM program. The author recommends that a search module be added in the future as an enhancement, of the RSM package. Another suggested enhancement is the addition of the Box and Behnken designs described in their 1960 paper (7) as another design type available to the user. Following this enhancement a thorough comparison of all offered designs needs to be accomplished to reveal the advantages and disadvantages of each design type as an RSM design. These recommended enhancements are proposed as a single research effort as much time is needed to gain the background knowledge that would be initially necessary.

## Appendix A. User Manual

Simulation models attempt to copy real, complex systems. As a result, the models themselves become very complex. The analyst wants to know what factors the simulation model is sensitive to, which factors have little impact on the output parameter of interest, the relationships between the input and output parameters, and the combination of input factors that produce the optimum response. The complex characteristics of simulation models makes necessary model analysis difficult.

The purpose of this program is to alleviate, to the maximum extent possible, a lot of the time and effort involved in setting up a simulation model for analysis. This computer program performs multidimensional sensitivity analysis by employing the techniques of response surface methodology interactively with a simulation model. The next section gives general information on response surface methodology techniques, and explains how to use this response surface methodology (RSM) computer program.

### RSM Theory

Response surface methodology is fundamentally a combination of statistical experimental design and regression analysis. The main problem addressed by RSM is to estimate, as closely as possible, the relationship between a response and the input factors implicitly defined within a process, by

experimentation with as few observations as possible. One main assumption of RSM is that this relationship can be expressed as a low order polynomial, i.e., a first or second order equation. An example of these kinds of equations are listed below,

first-order:  $Y=B_0 + B_1X_1 + \dots + B_kX_k$

second-order:  $Y=B_0 + B_1X_1 + \dots + B_kX_k + B_{11}X_1^2 + \dots + B_{kk}X_k^2 + B_{12}X_1X_2 + \dots + B_{k-1k}X_{k-1}X_k$

where k is the number of input factors. To estimate response surfaces, RSM employs designs that minimize the needed numbers of runs. The designs used to estimate first-order surfaces are the full  $2^k$  and the fractional  $2^k$ . For k factors, the full  $2^k$  requires  $2^k$  runs, and the fractional  $2^k$  requires a subset of the runs needed for the full  $2^k$ . The designs used to estimate second-order surfaces are the full  $3^k$ , the central composite design, and the fractional  $3^k$ . Table XVIII lists the designs offered by this computer program and the associated runs required depending on the number of factors to be tested. Care should be used in choosing the design type to use in program execution, because the number of runs required may become excessive.

#### Program Input

Program input requires only answering questions and following directions. Questions and input directions are discussed in the following paragraphs.

The first instruction displayed on the screen is,

TABLE XVIII

Number of Points Needed by Design Type

k	2	3	4	5	6	7	8	9
*full2k	4	8	16	32	64	128	256	512
*fractional 2k	4	8	8	8	8	8	16	32
**full3k	9	27	81	243	---	---	---	---
**CCD	16	23	36	36	59	100	100	177
**fractional 3k	9	27	81	81	243	243	243	243

\* first-order designs

\*\* second-order designs

Input the number of factors.

This instruction is self-explanatory, but this program is limited to handling only from two to nine factors. If any number outside of this interval is input, the screen displays,

The number of factors must be between  
2 and 9, inclusive.

Input the number of factors.

The next set of instructions obtains the maximum and minimum levels for each factor. The display for two factors is:

Input the maximum value for factor 1  
Input the minimum value for factor 1  
Input the maximum value for factor 2  
Input the minimum value for factor 2

Following this input, the user chooses the design type.  
Displayed as follows:

Input the design type you would like  
1--full 2\*\*k design  
2--fractional 2\*\*k design  
3--full 3\*\*k design  
4--central composite design  
5--fractional 3\*\*k design  
6--user inputted design

If 6 is entered, more input is required. This is discussed in an example later.



The next question to be answered by the user is:

How many repetitions would you like per observation?

The user inputs the number of repetitions desired. If the simulation model used is highly variable, more repetitions would be needed than if the model were not highly variable. Caution should be exercised before entering this value. If the design requires 20 observations, taken at different combinations of factor levels, and five repetitions are desired per observation, the total number of simulation runs required is 100. This many runs could require a great deal of computer time, depending on the complexity of the simulation model.

Next is the echo report of inputs, formatted as follows:

Your input k =

Design type =

Order of design =

Repetitions per run =

If any of these are incorrect, would you  
like to try again?

Type 1 for yes

Type 2 for no

At this time, if the user wants to change any of the inputs, the appropriate number is input.

The next display is:

Design matrix will be augmented with  
responses and written to file 'MATRIX'

with variables formatted consecutively

F12.5 with no spaces between.

Input the number for what you would like  
to do then:

1--continue with program to perform  
regression

2--stop program to perform regression  
with own package.

This computer program can perform the regression and obtain an estimate of the response surface dependent on the input factors, or the program can stop before executing the regression phase. In either case, the file 'MATRIX' is created and can be used for further analysis. The format is as written above and all but the last column is the design matrix. The columns of the design matrix represent the factors in the order in which they were input. The last column is the average response obtained from repetitions of simulation runs. Each row represents different combinations of factor levels and the associated response obtained.

This concludes the input required by the user.

#### Simulation Model Changes

Prior to running the response surface methodology program, several changes need to be made to the simulation model.

The program MAIN of the simulation model needs to be

changed to subroutine SIM with passed arguments (c,y1,j,k). C is the coded matrix which contains the factor levels to be used in the simulation runs, y1 is the response obtained for a run of the simulation model, j is the row of factor level combinations which are used on the present simulation run, and k is the number of factors to be varied.

The declarations for the variables which are passed need to be added to the simulation model main program which is now called the SIM subroutine.

Another addition to the SIM subroutine (previously program MAIN for the simulation model) is to establish the input levels for each of the factors before each run. Suppose the number of factors to be used is five and the names of these factors in the simulation model are fac1, fac2, fac3, fac4, and fac5. The coded matrix c contains the proper factor levels for each factor depending on the row of c to be run. The appropriate assignment statements to add are:

```
fac1 = c(j,1)
fac2 = c(j,2)
fac3 = c(j,3)
fac4 = c(j,4)
fac5 = c(j,5).
```

When the simulation model has completed a run, the response obtained needs to be transferred to y1. If the response is called output in the simulation model, the

correct assignment is:

y1 = output.

The obtained response from the simulation model is assigned to y1 which is passed back to the RSM program through the SIM subroutine arguments.

#### Problem Areas

There are problems that could occur depending on the computer system used and possible problems due to the RSM program and the simulation model now being one huge program. The open statements contained in the RSM program are in a format for the Vax 11/780. If the computer system used is different, checks of the open statements need to be made and changes made if necessary. The user also needs to check to ensure that all subroutines have unique names and also needs to check the arguments passed for the SIM subroutine to ensure that they are not used as different variables in the simulation model. If the simulation model is deterministic, the regression portion of the RSM program cannot be used because the pure error sum of squares will be zero and the program will attempt to divide by zero. In this case, the user should quit after the design matrix augmented with responses obtained from the simulation model is written to the file 'MATRIX'. The user can then use another statistical package to perform desired analysis.

#### Program Execution

After all the checks and needed changes of the RSM program and the simulation model have been made, these two files need to be merged into one. This file is the program that will be executed. Next the program needs to be compiled. The commands to perform the compilation will differ depending on the computer system used. Following program compilation, execution needs to be initiated. Again, this command will differ depending on the computer system used. After the execution command is given, the program will start by asking for user input which was discussed in an earlier section.

Tables XIX, XX, and XXI are examples of program execution in which the user wants to input his/her own design matrix. The user's answer follows each displayed question. The regression output the program displays will be discussed in the next section. Table XXII is the file 'MATRIX' that was generated by this RSM program.

#### Program Regression Output

Referring to the previous program input example, the number of factors to be tested is two, the design type desired is user input with six center points, and the user desires to perform the regression portion. Table XXIII illustrates the output from the regression portion.

The F-statistic for the regression model is 368.97 with degrees of freedom 6, 8. The critical value at an  $\alpha$ -level of .05 is 3.58. (33) This means that at a .05 significance

TABLE XIX  
Program Execution - 1

WELCOME TO THE  
  
INTERACTIVE RESPONSE SURFACE METHODOLOGY PACKAGE

written by  
1Lt Kalla J. Sparrow  
class of GOR-B4D

```
Input the number of factors
2
Input the maximum value for factor 1
100
Input the minimum value for factor 1
50
Input the maximum value for factor 2
240
Input the minimum value for factor 2
160
Input the design type you would like
1 -- full 2**k design
2 -- fractional 2**k design
3 -- full 3**k design
4 -- central composite design
5 -- fractional 3**k design
6 -- user inputted design
6
Have you read how to input your design matrix ?
If matrix is not inputted correctly this program will not work !
Type 1 to continue with user defined design matrix
Type 2 to return and rechoose design type
1
Input the order of your design
1 -- first order design
2 -- second order design
2
```

TABLE XX

Program Execution - 2

```

How many repetitions would you like per observation ?
1
You input k= 2
Design type= 6
Order of design= 2
Repetitions per run= 1
If any of these are incorrect would you like to try again?
Type 1 for yes
Type 2 for no
2
Design matrix will be augmented with responses and
written to file "matrix" with variables formatted
consecutively F12.5 with no spaces between.
Input the number for what you would like to do then:
1 -- continue with program to perform regression
2 -- stop program and perform regression with own
package
1
Remember to input all the columns including the
column for the intercept
If design is second-order you will need  $1+2k+(k(k-1))/2$ 
columns
If squared and interaction columns are not input in
the correct order the regression coefficients will
not be uncoded correctly.
Input the number of rows
14
Input the number of columns
6
The design matrix a is declared real
Input the center rows last!
Input the numbers with commas between them
Input row 1
1,-1,-1,1,1,1
Input row 2
1,-1,1,1,1,-1
Input row 3
1,1,-1,1,1,-1
Input row 4
1,1,1,1,1,1
Input row 5
1,-1.414,0,2,0,0
Input row 6
1,1.414,0,2,0,0
Input row 7

```

TABLE XXI

Program Execution - 3

```

1,0,-1.414,0,2,0
Input row 8
1,0,1.414,0,2,0
Input row 9
1,0,0,0,0,0
Input row 10
1,0,0,0,0,0
Input row 11
1,0,0,0,0,0
Input row 12
1,0,0,0,0,0
Input row 13
1,0,0,0,0,0
Input row 14
1,0,0,0,0,0
Here is your echo check

```

```

1.000-1.000-1.000 1.000 1.000 1.000
1.000-1.000 1.000 1.000 1.000-1.000
1.000 1.000-1.000 1.000 1.000-1.000
1.000 1.000 1.000 1.000 1.000 1.000
1.000-1.414 .000 2.000 .000 .000
1.000 1.414 .000 2.000 .000 .000
1.000 .000-1.414 .000 2.000 .000
1.000 .000 1.414 .000 2.000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000
1.000 .000 .000 .000 .000 .000

```

Input the # of center points in your design

6



TABLE XXII  
File 'MATRIX'

1.00000	-1.00000	-1.00000	1.00000	1.00000
1.00000	6276.72021			
1.00000	-1.00000	1.00000	1.00000	1.00000
-1.00000	4853.87012			
1.00000	1.00000	-1.00000	1.00000	1.00000
-1.00000	2661.69995			
1.00000	1.00000	1.00000	1.00000	1.00000
1.00000	3194.97998			
1.00000	-1.41400	.00000	2.00000	.00000
.00000	6386.47021			
1.00000	1.41400	.00000	2.00000	.00000
.00000	3112.44995			
1.00000	.00000	-1.41400	.00000	2.00000
.00000	3174.37988			
1.00000	.00000	1.41400	.00000	2.00000
.00000	3814.52002			
1.00000	.00000	.00000	.00000	.00000
.00000	3760.14990			
1.00000	.00000	.00000	.00000	.00000
.00000	3461.87988			
1.00000	.00000	.00000	.00000	.00000
.00000	3343.83008			
1.00000	.00000	.00000	.00000	.00000
.00000	3657.06006			
1.00000	.00000	.00000	.00000	.00000
.00000	3608.62012			
1.00000	.00000	.00000	.00000	.00000
.00000	3042.61011			

TABLE XXIII  
Regression Output

ANOVA for Response Surface Methodology

SOURCE	d.f.	SS	MS
Regression	6	227487600.000000	37914600.000000
Residual	8	822048.000000	102756.000000
Pure Error	5	336560.000000	67312.000000
Lack of Fit	3	485488.000000	161829.328125
Total	14	228309648.000000	

F-statistic for Regression Model= .368976990e+03 d.f.= 6 , 8

F-statistic for Lack of Fit= 2.40416765 d.f.= 3 , 5

Rsquare (corrected for mean) = .952540576e+00

degrees of freedom for t-statistics= 8

Beta Estimates	standard error(b)	t-statistic
b( 0)= 3479.02539	130.86635	26.58457
b( 1)= -1238.10889	113.34213	-10.92364
b( 2)= 1.94879	113.34213	.01719
b( 3)= 666.43396	117.96133	5.64960
b( 4)= 38.92819	117.96133	.33001
b( 5)= 489.03253	160.27788	3.05115

TABLE XXIII (CONT'D)

Regression Output

Uncoded Beta Estimates

```
-----
b(0)= .214902070e+05
b(1)= -307.2750244
b(2)= -46.3607712
b(1,1)= 1.0662943
b(2,2)= .0243301
b(1,2)= .4890325
```

-----  
Would you like to run this program again ?

Input 1 for yes or 2 for no

2

Thank you for using this Response Surface Methodology package  
Hopefully you obtained some useful information  
Have a nice day now !

level the regression model is significant.

The F-statistic for lack-of-fit is 2.404 with degrees of freedom 3, 5. At the  $\alpha=.05$  significance level the critical value is 5.41. (33) This means that lack-of-fit of the response surface due to higher order terms is not significant.

Rsquare represents the percentage of variation in the response explained by the included factors. Rsquare for this example is .95, i.e., 95% of the variation in the response is explained by the regression model.

The next section of Table XXIII gives the beta estimates, their standard errors, their t-statistics, and the degrees of freedom for the t-statistics. At an  $\alpha=.05$  significance level, the critical values for the t-statistic is  $T_{(.05,5)} = 2.015$ . (33) If the absolute value of the calculated t-statistic is smaller than the critical value, then one cannot reject the null hypothesis that the estimate is not significantly different from zero. Even though some of the beta estimates obtained may not be significantly different from zero, the increased adequacy of the estimated linear model by including these factors must be weighed against not including some of the factors which are not significantly different from zero. The estimated linear model for the response surface generated by the simulation is:

$$Y = 3479.03 - 1238.11X_1 + 1.95X_2 + 666.43X_1^2 + 38.93X_2^2 +$$

489.03X<sub>1</sub>X<sub>2</sub>.

And, as stated before, at a significance level of  $\alpha = .05$  the linear regression model is significant and does not exhibit a significant lack-of-fit. Also, 95% of the variation in the response is accounted for by the regression model.

The next output listed is the uncoded beta estimates. These estimates are in terms of the factor ranges inputted to be used in the simulation model. Over the inputted experimental region, the estimated regression model is:

$$Y_m = 21490.21 - 307.27X_1 - 46.36X_2 + 1.07X_1^2 + .02X_2^2 + .49X_1X_2.$$

This estimated equation gives a simple description of the response surface implicitly defined in the simulation model over the experimental region input. This equation can then be run into an optimization routine to determine that combination of factor levels that yields the optimum response. Also, a three-dimensional plot could be made to aid the user's understanding of the processes involved within the simulation model.

This user's guide describes the basic ideas involved in RSM and details the needed information so that the RSM program can be used in conjunction with a simulation model and yield beneficial information with little effort.

## Appendix B. Program Listing

\*PROGRAM NAME: main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:11 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*DESCRIPTION: This program performs response surface methodology  
 \* interactively with any FORTRAN based simulation model. First  
 \* after certain questions are answered by the user the proper design  
 \* matrix is generated. Then this matrix is translated to one which  
 \* the simulation model can interpret. When all the observations  
 \* have been taken a regression routine is run. Important  
 \* statistics and results are then printed to the screen and a  
 \* permanent file for the user's desired disposal is created with  
 \* the design matrix and the augmented response observations.  
 \* The user can then run any type of analysis desired on this file.  
 \* This program is organized in a structured manner; as such, the  
 \* main program is only the executive for the running of the  
 \* program.

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* time	integer	count number of times user runs package
* k	integer	# of factors to be included in analysis
* i	integer	used as loop counter
* dt	integer	design type
* ans	integer	answer to interactive question
* order	integer	order of design if user inputted
* rep	integer	# of repetitions to be run per row
* answ	integer	answer to interactive question
* res	integer	answer to interactive question
* m	integer	# of rows of design matrix
* n	integer	# of columns of design matrix
* aam	integer	# of rows of previous design matrix
* aan	integer	# of cols. of previous design matrix
* con	integer	answer to interactive question
* max(10)	real	maximum level for a factor
* min(10)	real	minimum level for a factor
* a(600,600)	real	design matrix
* aa(600,600)	real	previous used design matrix
* yave(600,600)	real	response average vector
* yyave(600,600)	real	previous response average vector
* c(600,600)	real	uncoded design matrix for simulation
* y(600,600)	real	response matrix obtained from sim
* b(600,600)	real	coded betas obtained in regression

```
*****
*****
```

```
*BEGINNING OF ACTUAL FORTRAN CODE*
```

```
program main
```

```
*DECLARATIONS*
```

```
integer time,k,i,dt,ans,order,rep,answ,res,m,n,aam,aan,con
real max(10),min(10),a(600,600),aa(600,600),yave(600,600),
+ yyave(600,600),c(600,600),y(600,600),b(600,600)
```

```
time=0
```

```

100 print 100
format(' /, ' /, ' /, ' /, ' /, ' /)
print *, '          WELCOME TO THE
print *
print *
print *
print *, 'INTERACTIVE RESPONSE SURFACE METHODOLOGY PACKAGE'
print *
print *
print *
print *, '          written by
print *
print *, '          1Lt Kalla J. Sparrow
print *
print *, '          class of GDR-84D
print 200
200 format(' /, ' /, ' /, ' /, ' /, ' /, ' /)
```

```
*****USER INPUT*****
```

```

3   print *, 'Input the number of factors'
    read *, k
    if (k .gt. 9 .or. k .lt. 2) then
        print *, 'The number of factors must be between'
        print *, '2 and 9, inclusive'
        go to 3
    endif
    do 1 i=1,k
        print *, 'Input the maximum value for factor ',i
        read *, max(i)
        print *, 'Input the minimum value for factor ',i
        read *, min(i)
1   continue
2   print *, 'Input the design type you would like'
    print *, '1 -- full 2**k design'
    print *, '2 -- fractional 2**k design'
    print *, '3 -- full 3**k design'
    print *, '4 -- central composite design'
```

```

print *, '5 -- fractional 3**k design'
print *, '6 -- user inputted design'
read *, dt
if (dt .eq. 6) then
    print *, 'Have you read how to input your design matrix ?'
    print *, 'If matrix is not inputted correctly this program',
+   'will not work !'
    print *, 'Type 1 to continue with user defined design matrix'
    print *, 'Type 2 to return and rechoose design type'
    read *, ans
    if (ans .eq. 2) then
        go to 2
    else
5      print *, 'Input the order of your design'
        print *, '1 -- first order design'
        print *, '2 -- second order design'
        read *, order
        if (order .ne. 1 .and. order .ne. 2) then
            print *, 'Design order is not correct'
            print *, 'Please try again'
            go to 5
        endif
    endif
endif

if (dt .ne. 1 .and. dt .ne. 2 .and. dt .ne. 3 .and. dt .ne. 4
+ .and. dt .ne. 5 .and. dt .ne. 6) then
    print *, 'You input the design type incorrectly'
    print *, 'Please try again'
    go to 2
endif

print *, 'How many repetitions would you like per observation ?'
read *, rep

print *, 'You input k= ', k
print *, 'Design type= ', dt
if (dt .eq. 6) then
    print *, 'Order of design= ', order
endif
print *, 'Repetitions per run= ', rep

print *, 'If any of these are incorrect would you like to',
+ ' try again?'
print *, 'Type 1 for yes'
print *, 'Type 2 for no'
read *, ans
if (ans .eq. 1) then
    go to 3
endif

print *, 'Design matrix will be augmented with responses and'
print *, 'written to file "matrix" with variables formatted '

```



```

    print *, 'consecutively F12.5 with no spaces between.'
7   print *, 'Input the number for what you would like to do then:'
    print *, '1 -- continue with program to perform regression'
    print *, '2 -- stop program and perform regression with own'
    print *, '    package'
    read *, res
    if (res .ne. 1 .and. res .ne. 2) then
        print *, 'Your answer was not correct. Try again.'
        go to 7
    endif

```

\*\*\*\*\*END OF USER INPUT\*\*\*\*\*

\*\*\*\*\*GENERATE DESIGN MATRIX\*\*\*\*\*

```

    if (dt .eq. 1) then
        call full2k(a,k,m,n)
    else if (dt .eq. 2) then
        call res3(a,k,m,n)
    else if (dt .eq. 3) then
        call full3k(a,k,m,n)
        if (k .gt. 5) then
            go to 2
        endif
    else if (dt .eq. 4) then
        call ccd(a,k,m,n)
    else if (dt .eq. 5) then
        call frac3k(a,k,m,n)
    else
        call user(a,k,m,n)
    endif

```

\*\*\*\*\*FINISHED GENERATING DESIGN MATRIX\*\*\*\*\*

```

    do 4 i=1,m
        yave(i,1)=0.
4   continue
    time=time+1

```

\*\*\*\* If this is more than the first time then need to compare  
 \*\*\*\* this design matrix with the previous one used. If some  
 \*\*\*\* of the rows are the same the response will be the same and  
 \*\*\*\* another response doesn't need to be obtained.

```

    if (time .gt. 1) then
        call compar(a,aa,m,n,aa,aa,yave,yyave)
    endif

```

\*\*\*\* Call the subroutine to code the design matrix into values  
 \*\*\*\* which the simulation model will be able to read.

```

    call code(a,c,m,k,min,max)

```

```

**** Call the subroutine which will run the simulation model
**** for those combinations of factor levels which need
**** to be obtained.

      call simrun(c,y,yave,m,k,rep)

**** Calculate the mean response for each combination of factor
**** levels.

      call mean(y,rep,m,yave)

**** Write the design matrix augmented with the average
**** responses to a file called 'matrix' to be used later
**** by the user.

      call write(a,yave,m,n)

      if (res .eq. 1) then
* user wants to perform the regression portion
        go to 1000
      else
* user wants to quit before regression portion of package begins
        go to 9999
      endif

**** Call the subroutine which performs the regression

1000  call regres(a,k,m,n,yave,dt,b)

**** Uncode the betas obtained for the design matrix into
**** the betas needed for the used factor levels.

      call uncode(b,min,max,dt,k,order)

**** Copy the design matrix used so will be able to compare
**** next generated matrix to see if there are some responses
**** which don't need to be obtained again. If there are
**** some combinations of factor levels which don't need
**** to be obtained again the average response will be contained
**** in the copied response vector.

      call copy(a,aa,m,n)
      call copy(yave,yyave,m,n)
      aa=m
      aa=n

10    print *, 'Would you like to run this program again ?'
      print *, 'Input 1 for yes or 2 for no'
      read *, con
      if (con .eq. 1) then
* user would like to run this program again
        go to 3
      else if (con .eq. 2) then

```

```

* user would not like to run this program again
  go to 9999
else
  print *, 'Your answer was incorrect. Try again.'
  go to 10
endif

9999 print *, 'Thank you for using this Response Surface Methodology',
+ ' package'
print *, 'Hopefully you obtained some useful information'
print *, 'Have a nice day now !'

end

```

```

*****
*****
*SUBROUTINE NAME: full2k

```

```

*ARGUMENT LIST: a,k,m,n
*CALLED BY      : main,res3,ccd

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE: sept 19

```

```

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

```

*****

```

```

*MODULE DESCRIPTION: This subroutine generates the full 2**k designs

```

```

*****

```

*ARGUMENTS:	IN/ * NAME	OUT	TYPE	PASSED/ GLOBAL	PURPOSE
* a(600,600)	out	real	passed	design matrix a	
* k	in/out	integer	passed	# of factors	
* m	out	integer	passed	# of rows of design	
* n	out	integer	passed	# of columns of design	

```

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
*col	integer	used as counter for columns
*row	integer	used as counter for rows
* r	integer	used as counter
* b	integer	used as counter
* j	integer	used as counter

```

*****
*****

```

```

*BEGINNING OF ACTUAL FORTRAN CODE*
  subroutine full2k(a,k,m,n)

```

```

*DECLARATIONS*
      integer col,row,k,m,n,r,b,j
      real a(600,600)
*ALGORITHM*

*calculate dimensions of the matrix
      m=2**k
      n=k+1
*initialize matrix
      do 1 row=1,2**k
        do 2 col=1,k+1
          a(row,col)=0.
2          continue
1      continue

*create first column of 1s
      do 3 row = 1,2**k
        a(row,1) = 1.
3      continue

*create rest of the columns for design
      do 4 col=2,k+1
        r=0
        b=2***(k+1-col)
        do 5 j=1,2***(col-2)
          do 6 row=r+1,r+b
            a(row,col)=-1.
6          continue
          do 7 row=r+b+1,r+2*b
            a(row,col)=1.
7          continue
          r=r+2*b
5        continue
4      continue

*add center point rows to be able to test for lack of fit
      do 8 row=1,4
        a(m+row,1)=1.
8      continue
      do 9 row=1,4
        do 10 col=2,k+1
          a(m+row,col)=0.
10     continue
9      continue

      m=m+4

      end
*****
*****

```

\*SUBROUTINE NAME:res3

\*ARGUMENT LIST:a,k,m,n

\*CALLED BY : main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:29 Sept

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION:subroutine to generate resolution III Fractional  
\* 2 k-p designs from rows of 1/16 of 2\*\*9 design matrix

\*\*\*\*\*

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* a(600,600)	out	real	passed	design matrix
* k	in/out	integer	passed	# of factors
* m	out	integer	passed	# of rows
* n	out	integer	passed	# of columns

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	used as row counter
* j	integer	used as column counter
* c(i,j)	real	rows from 1/16 of 2**9
* aa	integer	rows to copy
* i4(aa)	integer	used for data statement
* i5(aa)	integer	used for data statement
* i6(aa)	integer	used for data statement
* i7(aa)	integer	used for data statement
* i8(aa)	integer	used for data statement
* col	integer	used as counter

\*\*\*\*\*

\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

subroutine res3(a,k,m,n)

\*DECLARATIONS\*

integer i,j,aa,i4(17),i5(17),i6(17),col,k,m,n,  
+ i7(17),i8(17),row  
real c(600,600),a(600,600)

\*ALGORITHM\*

open(unit=7,file='resthree',status='old',access='sequential',  
+ form='formatted')  
rewind 7  
read(7,\*)((c(i,j),j=1,10),i=1,34)

```

if (k .eq. 2 .or. k .eq. 3) then
  call full2k(a,k,m,n)
  go to 2000
else if (k .eq. 4) then
  m=8
  n=5
  data(i4(aa),aa=1,8)/1,2,5,6,9,10,13,14/
  do 1 aa=1,m
    do 2 col=1,n
      a(aa,col)=c(i4(aa),col)
2      continue
1      continue

else if (k .eq. 5) then
  m=8
  n=6
  data(i5(aa),aa=1,8)/1,5,9,16,20,24,25,32/
  do 3 aa=1,m
    do 4 col=1,n
      a(aa,col)=c(i5(aa),col)
4      continue
3      continue

else if (k .eq. 6) then
  m=8
  n=7
  data(i6(aa),aa=1,8)/1,7,11,13,20,22,27,32/
  do 5 aa=1,m
    do 6 col=1,n
      a(aa,col)=c(i6(aa),col)
6      continue
5      continue

else if (k .eq. 7) then
  m=8
  n=8
  data(i7(aa),aa=1,8)/1,7,10,16,17,23,27,32/
  do 7 aa=1,m
    do 8 col=1,n
      a(aa,col)=c(i7(aa),col)
8      continue
7      continue

else if (k .eq. 8) then
  m=16
  n=9
  data(i8(aa),aa=1,16)/1,2,5,6,10,13,17,18,21,22,25,26,29,30,
+ 33,34/
  do 10 aa=1,16
    do 11 col=1,n
      a(aa,col)=c(i8(aa),col)
11      continue
10      continue

```

```

      else
*      k equals 9
          m=32
          n=10
          do 12 aa=1,m
              do 13 col=1,n
                  a(aa,col)=c(aa,col)
13              continue
12          continue

          endif

*add center point rows to be able to test for lack of fit
          do 14 row=1,4
              a(m+row,1)=1.
14          continue
          do 15 row=1,4
              do 16 col=2,k+1
                  a(m+row,col)=0.
16              continue
15          continue

          m=m+4

2000      end

```

```

*****
*****
*SUBROUTINE NAME: full3k

```

```

*ARGUMENT LIST: a,k,m,n
*CALLED BY      : main,frac3k

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE: 19 sept

```

```

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

```

*****

```

```

*MODULE DESCRIPTION: This subroutine generates the full 3*k designs

```

```

*****

```

*ARGUMENTS:	IN/ * NAME	OUT	TYPE	PASSED/ GLOBAL	PURPOSE
* a(600,600)	out		real	passed	generated design matrix
* k	in/out		integer	passed	# of factors
* m	out		integer	passed	# of rows of matrix
* n	out		integer	passed	# of columns of matrix

```

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
*col	integer	used for column counter
*row	integer	used for row counter
*nn	integer	used as counter for interaction columns
*cj	integer	used as counter for interaction cols.
*i	integer	used as counter
*j	integer	used as counter
*r	integer	used as increment for row counter
*b	integer	used as # of cycles for a given col
*jj	integer	used as counter for column generation

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

subroutine full3k(a,k,m,n)

\*DECLARATIONS\*

integer col,row,k,nn,cj,i,j,m,n,r,b,jj  
real a(600,600)

\* if k is greater than 5 then user cannot use this type of design

if (k .gt. 5) then

print\*, 'You input k = ', k

print\*, 'For k>5 the full3k design requires too many runs.'

print\*, 'Change your input design type to either 4 or 5.'

print\*, 'The CCD and Fractional 3\*\*k-p are more efficient.'

print\*, 'To change this limitation recode subroutine full3k.'

go to 1000

end if

\*ALGORITHM\*

\*calculate correct number of rows and columns

m=3\*\*k

n=1+2\*k+(k\*(k-1))/2

\*initialize design matrix

do 1 row=1,3\*\*k

do 2 col=1,1+2\*k+(k\*(k-1))/2

a(row,col)=0.

2 continue

1 continue

\*create first column of 1s

do 3 row = 1,3\*\*k

a(row,1) = 1.

3 continue

\*create rest of base design columns

do 4 col=2,k+1

r=0



```

        b=3*(k+1-col)
        do 5 jj=1,3*(col-2)
            do 6 row=r+1,r+b
                a(row,col)=-1.
6            continue
            do 7 row=r+b+1,r+(2*b)
                a(row,col)=0.
7            continue
            do 8 row=r+(2*b)+1,r+(3*b)
                a(row,col)=1.
8            continue
            r=r+(3*b)
5        continue
4    continue

*to generate next k columns square 2 through k+1 columns
    do 10 col = 2,k+1
        do 11 row = 1,3*k
            a(row,col+k) = a(row,col)*a(row,col)
11        continue
10    continue

*generate two-factor interaction columns
    nn = 2
    cj = 2
    do 12 i = 1,k-1
        do 13 j = cj,k
            do 14 row = 1,3*k
                a(row,2*k+nn) = a(row,i+1)*a(row,j+1)
14            continue
            nn = nn+1
13        continue
        cj=cj+1
12    continue

*create rows of center points to be able to calculate lack of fit
    do 15 row=1,4
        a(m+row,1)=1.
15    continue
    do 16 row=1,4
        do 17 col=2,1+2*k+(k*(k-1))/2
            a(m+row,col)=0.
17        continue
16    continue

    m=m+4

1000    end
*****
*****
*SUBROUTINE NAME:ccd
*ARGUMENT LIST:a,k,m,n

```

\*CALLED BY : main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:29 Sept

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: subroutine to generate resolution V fractional  
\* 2\*\*k-p designs for base of ccd designs -- then adds rows of axial  
\* or star points -- then adds rows of center points

\*\*\*\*\*

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* a(600,600)	out	real	passed	design matrix
* k	in/out	integer	passed	# of factors
* m	out	integer	passed	# of rows
* n	out	integer	passed	# of columns

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* row	integer	used as row counter
* col	integer	used as column counter
* mm	integer	used as # of rows
* i	integer	used as counter
* j	integer	used as counter
* aa	integer	used as counter for data
* i5(aa)	integer	array for data
* i6(aa)	same	same
* i7(aa)	same	same
* i8(aa)	same	same
* nn	integer	used as counter
* cj	integer	used as counter
* c(m,n)	real	design matrix
* alpha	real	constant for axial rows

\*\*\*\*\*

\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

subroutine ccd(a,k,m,n)

\*DECLARATIONS\*

integer k,m,n,row,col,mm,i,j,aa,i5(65),i6(65),i7(65),nn,cj,  
+ i8(65)  
real c(600,600),alpha,a(600,600)

open(unit=7,file='resfive',status='old',access='sequential',  
+ form='formatted')  
rewind 7

```

      read(7,*)((c(i,j),j=1,10),i=1,128)

*initialize biggest matrix will need
      do 1 row=1,600
        do 2 col=1,600
          a(row,col)=0.
2        continue
1      continue

      if (k .eq. 2) then
        call full2k(a,2,n)
        m=2*k
        alpha=2*(k/4.)
* build first col of 1s for axial rows and center point rows
        do 3 row=m+1,m*2*k+8
          a(row,1)=1.
3        continue
* add rows of axial (star) points
        mm=m
        do 4 col=2,k+1
          a(mm+1,col)=-alpha
          a(mm+2,col)=alpha
          mm=mm+2
4        continue
        m=m+2*k+8
        n=1+2*k+(k*(k-1))/2

      else if (k .eq. 3) then
        call full2k(a,3,n)
        m=2*k
        alpha=2*(k/4.)
* build first col of 1s for axial rows and center point rows
        do 5 row=m+1,m+2*k+9
          a(row,1)=1.
5        continue
* add rows of axial (star) points
        mm=m
        do 6 col=2,k+1
          a(mm+1,col)=-alpha
          a(mm+2,col)=alpha
          mm=mm+2
6        continue
        m=m+2*k+9
        n=1+2*k+(k*(k-1))/2

      else if (k .eq. 4) then
        call full2k(a,4,n)
        m=2*k
        alpha=2*(k/4.)
* build first col of 1s for axial rows and center point rows
        do 7 row=m+1,m+2*k+12
          a(row,1)=1.
7        continue

```

```

* add rows of axial (star) points
      mm=m
      do 8 col=2,k+1
        a(mm+1,col)=-alpha
        a(mm+2,col)=alpha
        mm=mm+2
8      continue
      m=m+2*k+12
      n=1+2*k+(k*(k-1))/2

      else if (k .eq. 5) then
        m=16
        n=6
        data(i5(aa),aa=1,16)/1,3,5,6,7,10,12,14,66,68,70,72,
+        73,75,77,79/
* build base part of design
      do 9 aa=1,m
        do 10 col=1,n
          a(aa,col)=c(i5(aa),col)
10      continue
9      continue
      alpha=2**((k-1)/4.)
* build first col of 1s for axial rows and center point rows
      do 11 row=m+1,m+2*k+10
        a(row,1)=1.
11      continue
* add rows of axial (star) points
      mm=m
      do 12 col=2,k+1
        a(mm+1,col)=-alpha
        a(mm+2,col)=alpha
        mm=mm+2
12      continue
      m=m+2*k+10
      n=1+2*k+(k*(k-1))/2

      else if (k .eq. 6) then
        m=32
        n=7
        data(i6(aa),aa=1,32)/1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,
+        65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80/
* build base part of design
      do 13 aa=1,m
        do 14 col=1,n
          a(aa,col)=c(i6(aa),col)
14      continue
13      continue
      alpha=2**((k-1)/4.)
* build first col of 1s for axial rows and center point rows
      do 15 row=m+1,m+2*k+15
        a(row,1)=1.
15      continue
* add rows of axial (star) points

```

```

      aa=a
      do 16 col=2,k+1
        a(aa+1,col)=-alpha
        a(aa+2,col)=alpha
        aa=aa+2
16      continue
      m=m+2*k+15
      n=1+2*k+(k*(k-1))/2

      else if (k .eq. 7) then
        m=64
        n=8
        data(i7(aa),aa=1,64)/1,4,5,8,9,12,13,16,18,19,22,23,26,27,
+      30,31,33,36,37,40,41,44,45,48,50,51,54,55,58,59,62,63,
+      66,67,70,71,74,75,78,79,81,84,85,88,89,92,93,96,98,99,
+      102,103,106,107,110,111,113,116,117,120,121,124,125,128/
      * build base part of design
      do 17 aa=1,m
        do 18 col=1,n
          a(aa,col)=c(i7(aa),col)
18        continue
17      continue
      alpha=2*((k-1)/4.)
      * build first col of 1s for axial rows and center point rows
      do 19 row=m+1,m+2*k+22
        a(row,1)=1.
19      continue
      * add rows of axial (star) points
      aa=a
      do 20 col=2,k+1
        a(aa+1,col)=-alpha
        a(aa+2,col)=alpha
        aa=aa+2
20      continue
      m=m+2*k+22
      n=1+2*k+(k*(k-1))/2

      else if (k .eq. 8) then
        m=64
        n=9
        data(i8(aa),aa=1,64)/1,2,3,4,9,10,11,12,21,22,23,24,29,30,
+      31,32,33,34,35,36,41,42,43,44,53,54,55,56,61,62,63,64,65,
+      66,67,68,73,74,75,76,85,86,87,88,93,94,95,96,97,98,99,
+      100,105,106,107,108,117,118,119,120,125,126,127,128/
      * build base part of design
      do 21 aa=1,m
        do 22 col=1,n
          a(aa,col)=c(i8(aa),col)
22        continue
21      continue
      alpha=2*((k-2)/4.)
      * build first col of 1s for axial rows and center point rows
      do 23 row=m+1,m+2*k+20

```

```

        a(row,1)=1.
23      continue
* add rows of axial (star) points
        mm=m
        do 24 col=2,k+1
            a(mm+1,col)=-alpha
            a(mm+2,col)=alpha
            mm=mm+2
24      continue
        m=m+2*k+20
        n=1+2*k+(k*(k-1))/2

        else
* k equals 9
        m=128
        n=10
* build base part of design
        do 25 aa=1,m
            do 26 col=1,n
                a(aa,col)=c(aa,col)
26          continue
25      continue
        alpha=2*((k-2)/4.)
* build first col of 1s for axial rows and center point rows
        do 27 row=m+1,m+2*k+31
            a(row,1)=1.
27      continue
* add rows of axial (star) points
        mm=m
        do 28 col=2,k+1
            a(mm+1,col)=-alpha
            a(mm+2,col)=alpha
            mm=mm+2
28      continue
        m=m+2*k+31
        n=1+2*k+(k*(k-1))/2
    endif

* to generate next k columns square 2 through k+1 columns
        do 29 col=2,k+1
            do 30 row=1,m
                a(row,col+k)=a(row,col)*a(row,col)
30          continue
29      continue

* generate two-factor interaction columns
        nn=2
        cj=2
        do 31 i=1,k-1
            do 32 j=cj,k
                do 33 row=1,m
                    a(row,2*k+nn)=a(row,i+1)*a(row,j+1)
33          continue

```

```

nn=nn+1
32    continue
    cj=cj+1
31    continue

end

```

```

*****
*****
*SUBROUTINE NAME: frac3k

```

```

*ARGUMENT LIST:a,k,m,n
*CALLED BY    : main

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:29 Sept

```

```

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

```

*****

```

```

*MODULE DESCRIPTION:subroutine which generates the fractional 3**k-p
* designs used to estimate second order equations

```

```

*****

```

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* a(600,600)	out	real	passed	generated design matrix
* k	in/out	integer	passed	# of factors
* m	out	integer	passed	# rows of design matrix
* n	out	integer	passed	# cols of design matrix

```

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* row	integer	used as a row counter
* i	integer	used as a counter
* j	integer	used as a counter
* col	integer	used as a column counter
* nn	integer	counter used to make interaction cols
* cj	integer	counter used to make interaction cols
* ii	integer	counter used to make interaction cols
* jj	integer	counter used to make interaction cols
* rn5(250)	integer	data statement array for rows
* rn6(250)	integer	data statement array for rows
* rn7(250)	integer	data statement array for rows
* rn8(250)	integer	data statement array for rows
* rn9(250)	integer	data statement array for rows

```

*****
*****

```

```

*BEGINNING OF ACTUAL FORTRAN CODE*

```

```

subroutine frac3k(a,k,m,n)

*DECLARATIONS*
  integer k,m,n,row,i,j,col,nn,cj,ii,jj,rn5(250),rn6(250),
+   rn7(250),rn8(250),rn9(250)
  real a(600,600)

*ALGORITHM*
* calculate # of columns of complete design matrix
  n=1+2*k+(k*(k-1))/2

* depending on the # of factors determine which rows will be included

  if (k .eq. 2 .or. k .eq. 3 .or. k .eq. 4) then
    call full3k(a,k,m,n)
    go to 2000

  else if (k .eq. 5) then
    m=81
    data(rn5(row),row=1,81)/1,6,8,12,14,17,20,22,27,30,32,34,
+   38,40,45,46,51,53,56,58,63,64,69,71,75,77,79,84,86,89,92,
+   94,99,100,105,107,110,112,117,118,123,125,129,131,133,136,
+   141,143,147,149,151,155,157,162,164,166,171,172,177,179,
+   183,185,187,190,195,197,201,203,205,209,211,216,219,221,
+   223,227,229,234,235,240,242/
* build first column of 1s
    do 1 row=1,m
      a(row,1)=1.
1    continue

* build base design
    do 2 row=1,m
      do 3 j=1,k
        do 4 i=1,3
          if (rn5(row) .le. i*(3*(k-j))) then
            a(row,j+1)=i-2
            rn5(row)=rn5(row)-(i-1)*3*(k-j)
            go to 3
          endif
4        continue
3      continue
2    continue

  else if (k .eq. 6) then
    m=243
    data(rn6(row),row=1,243)/1,367,724,348,678,72,665,50,380,
+   493,121,478,102,441,555,419,533,143,247,604,241,594,195,
+   309,173,296,626,139,415,538,486,492,120,551,107,437,622,
+   178,292,240,246,612,314,590,191,385,661,46,723,9,366,68,
+   344,683,196,310,586,291,630,177,608,236,251,679,64,349,
+   54,384,660,362,728,5,433,556,103,537,138,423,125,482,488,
+   254,620,221,571,199,322,189,276,633,17,374,704,325,691,
+   76,672,30,396,500,128,467,88,445,559,426,522,150,392,668,

```



```

k      35,709,13,370,75,333,690,146,431,518,463,496,133,567,87,
+      444,638,185,272,217,259,616,321,570,207,449,563,83,514,
+      151,427,132,462,504,203,317,575,277,634,181,615,225,258,
+      686,80,329,31,388,673,378,708,12,507,117,474,95,452,548,
+      412,526,154,270,600,228,578,215,302,166,280,646,24,354,
+      720,341,698,56,649,43,400,645,165,288,233,266,596,298,
+      583,211,399,657,42,716,20,359,61,337,694,162,411,525,470,
+      512,113,544,91,457,702,60,336,38,404,653,355,712,25,456,
+      543,99,530,158,407,109,475,508,210,306,582,284,641,170,
+      601,229,262/
* build first column of 1s
  do 6 row=1,m
    a(row,1)=1.
6    continue

* build base design
  do 7 row=1,m
    do 8 j=1,k
      do 9 i=1,3
        if (rn6(row) .le. i*(3**(k-j))) then
          a(row,j+1)=i-2
          rn6(row)=rn6(row)-(i-1)*3**(k-j)
          go to 8
        endif
      9    continue
    8    continue
  7    continue

  else if (k .eq. 7) then
    m=243
    data(rn7(row),row=1,115)/1,1357,1894,1967,398,944,990,
+    1608,687,1587,675,1050,1336,1873,70,359,896,2000,956,
+    1988,338,708,1002,1548,1942,49,1315,8,1355,1892,1965,
+    405,942,985,1603,691,1591,670,1045,1334,1880,68,357,
+    894,2007,963,1986,336,703,1006,1543,1940,47,1322,6,
+    1353,1899,1969,400,937,983,1610,689,1589,668,1052,1341,
+    1878,66,352,898,2002,958,1981,340,710,1004,1541,1938,
+    54,1320,472,766,2041,1682,518,1055,1452,1755,105,1707,
+    138,1413,754,2101,451,497,1124,1661,1103,1640,566,126,
+    1392,1767,2053,412,787,470,773,2039,1680,516,1062,1456/
    data(rn7(row),row=116,243)/1750,
+    100,1702,142,1408,752,2099,458,504,1122,1659,1101,
+    1647,564,121,1387,1771,2060,410,785,477,771,2037,1675,
+    520,1057,1454,1748,107,1709,140,1406,750,2106,456,499,
+    1117,1663,1105,1642,559,119,1394,1769,2058,408,792,
+    619,1156,1531,1820,179,1283,843,2109,306,2178,285,822,
+    1189,1492,571,239,1262,1808,1223,1841,191,264,891,2157,
+    1471,631,1177,617,1154,1538,1827,177,1281,838,2113,301,
+    2173,280,826,1196,1490,569,237,1269,1806,1221,1839,198,
+    268,886,2152,1469,638,1175,615,1161,1536,1822,172,1285,
+    845,2111,299,2171,287,824,1194,1488,576,241,1264,1801,
+    1216,1843,193,266,884,2159,1476,636,1173/

```

```

* build first column of 1s
  do 11 row=1,m
    a(row,1)=1.
11  continue

* build base design
  do 12 row=1,m
    do 13 j=1,k
      do 14 i=1,3
        if (rn7(row) .le. i*(3*(k-j))) then
          a(row,j+1)=i-2
          rn7(row)=rn7(row)-(i-1)*3*(k-j)
          go to 13
        endif
      continue
    13  continue
  12  continue

  else if (k .eq. 8) then
    m=243
    data(rn8(row),row=1,147)/1,1093,2185,2585,3569,3689,
+ 5061,5181,6165,2740,3022,4078,4487,5579,6338,429,1251,
+ 1605,4669,5725,6007,584,938,1760,2412,3171,4263,1717,
+ 613,949,4274,2360,3209,6048,4674,5685,3718,2515,3607,
+ 6194,5099,5111,2109,42,1134,6349,4525,5527,1562,440,
+ 1280,4119,2700,3027,1237,1573,469,3065,4076,2702,5541,
+ 6390,4476,3220,4222,2398,5723,6050,4631,909,1749,627,
+ 5140,6232,5029,1055,2147,80,3639,3651,2556,1507,385,
+ 1387,3983,2888,2972,6540,4392,5475,4138,2305,3397,
+ 5993,4781,5630,1908,561,816,6139,4963,5299,2054,230,
+ 998,3828,2463,3555,1000,2092,187,3503,3839,2501,5331,
+ 6099,4977,2929,4021,2890,5486,6497,4421,1428,1521,
+ 336,5668,5914,4819,854,1937,491,3330,4170,2346,529,
+ 883,1867,2276,3359,4208,4860,5592,5955,2449,3514,3877/
    data(rn8(row),row=148,243)/5006,
+ 5288,6110,192,1041,2052,4432,5443,6526,374,1439,
+ 1469,2850,2970,4026,799,1801,679,3275,4358,2210,5778,
+ 5862,4767,3448,3784,2608,5195,6287,4922,1191,1959,
+ 135,5350,6442,4609,1373,1628,281,3120,3969,2757,319,
+ 1303,1657,2795,3158,3890,4542,5391,6474,2221,3304,4315,
+ 4724,5780,5900,720,750,1815,4870,5233,6298,137,1148,
+ 1997,2640,3462,3744,1999,94,1186,3773,2651,3419,6249,
+ 4911,5247,3928,2833,3079,6404,4580,5420,1698,252,1335,
+ 5857,4726,5818,1853,668,761,4329,2253,3264/

* build first column of 1s
  do 16 row=1,m
    a(row,1)=1.
16  continue

* build base design
  do 17 row=1,m
    do 18 j=1,k

```

```

do 19 i=1,3
  if (rn8(row) .le. i*(3**k-j)) then
    a(row,j+1)=i-2
    rn8(row)=rn8(row)-(i-1)*3**k-j
    go to 18
  endif
19   contiNue
18   continue
17   continue

  else
* k equals 9
    m=243
    data(rn9(row),row=1,125)/1,14279,8604,9193,3518,16815,
+ 18142,11729,6297,4215,15331,9899,12435,4813,18839,15066,
+ 7192,788,5510,19545,10951,7898,1494,13573,16118,10677,
+ 2812,3163,17441,8841,12355,5942,17790,14005,8330,711,
+ 4461,18493,13052,6849,1405,14711,16032,9625,3950,2111,
+ 13230,7543,10331,2460,16735,19271,11652,5245,6325,17678,
+ 12003,8218,356,14391,17167,9305,3135,1062,15085,6737,
+ 10002,3838,15686,18465,12787,4916,2357,16383,10705,
+ 11297,5622,19168,13685,7524,1837,12232,5855,17919,13891,
+ 8459,615,3400,17399,8808,6969,1318,14597,15918,9511,
+ 4097,4455,18694,13019,10208,2616,16621,19400,11538,5149,
+ 2105,13188,7753,8104,269,14511,17053,9425,3048,6553,
+ 17645,11970,10131,3751,15563,18351,12664,5072,1047,13295/
    data(rn9(row),row=126,243)/6704,
+ 11183,5778,19045,13814,7401,1750,2342,16350,10915,
+ 9079,3422,16944,18019,11858,6210,238,14246,8562,12564,
+ 4717,18725,14943,7078,944,4209,15541,9857,7784,1641,13459,
+ 16238,10563,2725,5504,19512,11152,17173,9338,2934,6439,
+ 17531,12117,8098,470,14478,18228,12820,4958,1176,15181,
+ 6608,10125,3709,15773,13691,7314,1879,2228,16479,10819,
+ 11420,5736,19012,18148,11771,6087,124,14123,8718,9064,
+ 3632,16911,14829,7234,821,4338,15418,9770,12549,4684,
+ 18935,16124,10476,2845,5390,19632,11065,8012,1608,13426,
+ 14020,8363,501,3277,17285,8964,12226,6065,17877,15804,
+ 9658,3983,4575,18580,12932,6963,1285,14798,19286,11442,
+ 5278,1982,13317,7666,10445,2583,16579/

* build first column of 1s
  do 21 row=1,m
    a(row,1)=1.
21   continue

* build base design
  do 22 row=1,m
    do 23 j=1,k
      do 24 i=1,3
        if (rn9(row) .le. i*(3**k-j)) then
          a(row,j+1)=i-2
          rn9(row)=rn9(row)-(i-1)*3**k-j
          go to 23
        endif
      enddo
    enddo
  enddo

```

```

                endif
24         continue
23     continue
22 continue

    endif

* build squared columns
1000 do 26 col=2,k+1
        do 27 row=1,m
            a(row,col+k)=a(row,col)*a(row,col)
27         continue
26     continue

* build two-factor interaction columns
    nn=2
    cj=2
    do 28 ii=1,k-1
        do 29 jj=cj,k
            do 30 row=1,m
                a(row,2*k+nn)=a(row,ii+1)*a(row,jj+1)
30             continue
            nn=nn+1
29         continue
        cj=cj+1
28     continue

*create rows of center points to be able to calculate lack of fit
    do 31 row=1,4
        a(m+row,1)=1.
31     continue
    do 32 row=1,4
        do 33 col=2,1+2*k+(k*(k-1))/2
            a(m+row,col)=0.
33         continue
32     continue

    m=m+4

2000 end

*****
*****
*SUBROUTINE NAME: user

*ARGUMENT LIST: (a,k,m,n)
*CALLED BY      : main

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

\*\*\*\*\*

\*MODULE DESCRIPTION: This subroutine asks the user to input his own  
\* design matrix

\*\*\*\*\*

*ARGUMENTS:	IN/ * NAME	TYPE DUT	PASSED/ GLOBAL	PURPOSE
* a(600,600)	out	real	passed	inputted design matrix
* k	in	integer	passed	the # of factors
* m	out	integer	passed	the # of rows of a
* n	out	integer	passed	the # of cols. of a

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	used for a row counter in do loop
* j	integer	used for a column counter in loop

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*  
subroutine user(a,k,m,n)

\*DECLARATIONS\*

integer m,n,k,i,j  
real a(600,600)

print \*, 'Remember to input all the columns including the'  
print \*, 'column for the intercept'  
print \*, 'If design is second-order you will need 1+2k+(k(k-1))/2'  
print \*, 'columns'  
print \*, 'If squared and interaction columns are not input in'  
print \*, 'the correct order the regression coefficients will'  
print \*, 'not be uncoded correctly.'  
print \*, 'Input the number of rows'  
read \*, m  
print \*, 'Input the number of columns'  
read \*, n  
print \*, 'The design matrix a is declared real'

print \*, 'Input the center rows last!'  
print \*, 'Input the numbers with commas between them'  
do 1 i=1,m  
print \*, 'Input row ', i  
read \*, (a(i,j), j=1,n)

1 continue

print \*, 'Here is your echo check'  
print \*

```

      print *
      print *
      print *
      print *
      print *
      print *
      do 2 i=1,m
        print 100,(a(i,j),j=1,n)
100    format(' ',11F6.3/(' ',11F6.3)/(' ',11F6.3)/(' ',11F6.3)/
      +      (' ',11F6.3))
2      continue

      end

```

```

*****
*****
*SUBROUTINE NAME: compar

```

```

*ARGUMENT LIST: (a,aa,m,n,aam,aan,yave,yyave)
*CALLED BY      : main

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

```

```

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

```

*****

```

```

*MODULE DESCRIPTION: This subroutine compares two matrices -- the
* most recent generated design matrix (a) and the previously
* used design matrix (aa). If there are rows that are the same
* then the response average will be the same. The simulation model
* does not need to be run for that row. The previously obtained
* response can be copied into the response average vector for this
* most recent matrix and be used for the regression.

```

```

*****

```

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* a(600,600)	in	real	passed	recent design matrix
* aa(600,600)	in	real	passed	previous design matrix
* m	in	integer	passed	# of rows of a
* n	in	integer	passed	# of columns of a
* aam	in	integer	passed	# of rows of aa
* aan	in	integer	passed	# of columns of aa
* yave(600,600)	out	real	passed	response averages that
*				are the same
* yyave(600,600)	in	real	passed	response averages from
*				the previous analysis

```

*****

```

```

*LOCAL VARIABLES:      TYPE:      PURPOSE:

```

```

* i            integer    used as row counter for a
* j            integer    used as column counter for a
* k            integer    used as row counter for aa
* r(600)       integer    used for nonrepeated rows

```

```

*****
*****

```

```

*BEGINNING OF ACTUAL FORTRAN CODE*

```

```

subroutine compar(a,aa,m,n,aa,aa,yave,yyave)

```

```

*DECLARATIONS*

```

```

integer m,n,aa,aa,i,j,k,r(600)
real a(600,600),aa(600,600),yave(600,600),yyave(600,600)

```

```

do 1 i=1,m
  k=1
10  if (a(i,1) .eq. aa(k,1)) then
    go to 3
  else
    k=k+1
    go to 10
  endif

3  do 2 j=2,n
    if (a(i,j) .eq. aa(k,j)) then
      if (j .ne. n+1) then
        go to 2
      else
        if (r(k) .eq. 1) then
          go to 1
        else
          yave(i,1)=yyave(k,1)
          r(k)=1
          go to 1
        endif
      endif
    else
      go to 1
    endif
  endif
2  continue
1  continue

end

```

```

*****
*****

```

```

*SUBROUTINE NAME: code

```

```

*ARGUMENT LIST: (a,c,m,k,min,max)

```

```

*CALLED BY : main

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

```

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: This subroutine codes the design matrix into  
\* a matrix (c) that has the factors at the levels needed for  
\* the simulation model.

\*\*\*\*\*

*ARGUMENTS:	IN/ # NAME	TYPE	PASSED/ GLOBAL	PURPOSE
	# a(600,600)	in real	passed	design matrix
	# c(600,600)	out real	passed	coded design matrix
	# m	in integer	passed	# of rows of both
	# k	in integer	passed	# of factors
	# min(10)	in real	passed	minimum for each factor
	# max(10)	in real	passed	maximum for each factor

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
# i	integer	used for counter to compute ranges and averages for each factor
# j	integer	used for row counter
# l	integer	used for column counter
# range(10)	real	range of each factor
# ave(10)	real	average of each factor

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*  
subroutine code(a,c,m,k,min,max)

\*DECLARATIONS\*  
integer m,k,i,j,l  
real max(10),min(10),range(10),ave(10),a(600,600),c(600,600)

\* calculate range and average of each factor  
do 1 i=1,k  
range(i)=max(i)-min(i)  
ave(i)=(max(i)+min(i))/2.  
1 continue

\* code matrix c to inputs that simulation model can accept  
do 2 j=1,m  
do 3 l=1,k  
c(j,l)=a(j,l+1)\*range(l)/2.+ave(l)  
3 continue  
2 continue



end

\*\*\*\*\*  
\*\*\*\*\*  
\*SUBROUTINE NAME: simrun

\*ARGUMENT LIST: (c,y,yave,m,k,rep)  
\*CALLED BY : main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: This subroutine calls the sim subroutine  
\* written by the user to obtain responses for those rows needed.

\*\*\*\*\*

*ARGUMENTS:	IN/ * NAME	TYPE OUT	PASSED/ GLOBAL	PURPOSE
* c(600,600)	in	real	passed	coded matrix of factor levels
* y(600,600)	out	real	passed	matrix of responses
* yave(600,600)	in	real	passed	previously obtained responses
* m	in	integer	passed	# of rows of c
* k	in	integer	passed	# of factors
* rep	in	integer	passed	# of replications

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* j	integer	row you are on in c
* l	integer	repetition you are on in row j
* yl	real	an observation that is obtained

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*  
subroutine simrun(c,y,yave,m,k,rep)

\*DECLARATIONS\*  
integer m,k,j,l,rep  
real c(600,600),y(600,600),yave(600,600),yl  
  
do 1 j=1,m  
if (yave(j,1) .ne. 0.) then  
go to 1

```

        else
          do 2 l=1,rep
            call sim(c,y1,j,k)
            y(j,l)=y1
2          continue
        endif
1      continue

    end

```

```

*****
*****

```

\*SUBROUTINE NAME: mean

\*ARGUMENT LIST: (y,rep,m,yave)

\*CALLED BY : main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

*****

```

\*MODULE DESCRIPTION: This subroutine calculates the mean of each row  
\* of a matrix

```

*****

```

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* y(600,600)	in	real	passed	matrix of responses
* rep	in	integer	passed	# of repetitions
* m	in	integer	passed	# of rows of y
* yave(600,600)	out	real	passed	matrix of averages

```

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	counter used for rows
* j	integer	counter used for columns
* sum	real	used to calculate rsum

```

*****
*****

```

\*BEGINNING OF ACTUAL FORTRAN CODE\*  
subroutine mean(y,rep,m,yave)

\*DECLARATIONS\*  
integer rep,i,j,m  
real y(600,600),yave(600,600),sum

```

      do 1 i=1,m
        if (yave(i,1) .ne. 0) then
          go to 1
        else
          sum=0.
          do 2 j=1,rep
            sum=sum+y(i,j)
2          continue
          yave(i,1)=sum/rep
        endif
1      continue

      end

```

```

*****
*****
*SUBROUTINE NAME: write

```

```

*ARGUMENT LIST: (a,yave,m,n)
*CALLED BY      : main

```

```

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:10 October

```

```

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

```

*****
*MODULE DESCRIPTION: This subroutine writes the design matrix a
* augmented with the response vector yave to a permanent file
* matrix to be used in a statistical package of the user's choice.

```

```

*****
*ARGUMENTS:      IN/   TYPE      PASSED/   PURPOSE
* NAME           OUT          GLOBAL
* a(600,600)    in    real      passed     design matrix
* yave(600,600) in    real      passed     response vector
* m             in    integer    passed     # of rows of a and yave
* n             in    integer    passed     # of columns of a

```

```

*****
*LOCAL VARIABLES: TYPE:      PURPOSE:
* i               integer    used as row counter in write
* j               integer    used as column counter in write
* l               integer    used to augment a and yave

```

```

*****
*****
*BEGINNING OF ACTUAL FORTRAN CODE*
      subroutine write(a,yave,m,n)

```

```

*DECLARATIONS*
  integer m,n,i,j,l
  real a(600,600),yave(600,600)

  open(unit=7,file='matrix',status='new',access='sequential',
+  form='formatted')
  rewind 7

  do 3 l=1,m
    a(l,n+1)=yave(l,1)
3  continue

  do 1 i=1,m
    write(7,100)(a(i,j),j=1,n+1)
100  format(' ',5F12.5/(' ',5F12.5)/(' ',5F12.5)/
+  (' ',5F12.5)/(' ',5F12.5)/(' ',5F12.5)/(' ',5F12.5)/
+  (' ',5F12.5)/(' ',5F12.5)/(' ',5F12.5)/(' ',5F12.5)/
+  (' ',5F12.5))
1  continue

  end

*****
*****
*SUBROUTINE NAME: regres

*ARGUMENT LIST: (x,k,m,n,y,dt,b)
*CALLED BY      : main

*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:9 October

*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

*****

*MODULE DESCRIPTION: This subroutine performs the regression by use
* of least squares procedure

*****

*ARGUMENTS:      IN/   TYPE      PASSED/   PURPOSE
* NAME           OUT                                GLOBAL
* x(600,600)     in    real       passed     design matrix a
* k              in    integer    passed     # of factors
* m              in    integer    passed     # of rows of x or a
* n              in    integer    passed     # of cols of x or a
* y(600,600)     in    real       passed     response vector
* dt             in    integer    passed     design type
* b(600,600)     out   real       passed     beta estimates(coded)

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	used as do loop counter
* j	integer	used as do loop counter
* regdf	integer	regression degrees of freedom
* resdf	integer	residual degrees of freedom
* totdf	integer	total degrees of freedom
* pedf	integer	pure error degrees of freedom
* lacdf	integer	lack of fit degrees of freedom
* nl	integer	# of replicated center points
* c(600,600)	real	matrix obtained from matmul
* v(60,60)	real	variance-covariance matrix
* srot(60)	real	standard errors of coefficients
* t(60)	real	t-statistics for coefficients
* sum	real	used to compute ybar
* rsq	real	r squared statistic
* freg	real	f-statistic for regression
* flac	real	f-statistic for lack of fit
* SSreg	real	sum of squares due to regression
* MSreg	real	mean squares due to regression
* SSregc	real	SSreg corrected for mean
* SSres	real	sum of squares due to residual
* MSres	real	mean squares due to residual
* SStot	real	total sum of squares
* SStotc	real	SStot corrected for mean
* SSpe	real	sum of squares due to pure error
* MSpe	real	mean squares due to pure error
* SSlac	real	sum of squares due to lack of fit
* MSlac	real	mean squares due to lack of fit
* ccc(600,600)	real	used in matmul subroutine
* cc(600,600)	real	used in matmul subroutine
* ybar	real	average of responses
* sumc	real	used to compute ybar of center points
* ybarc	real	average of responses at center points
* yy	real	used to calculate y'y at center pts.
* btran(600,600)	real	b transpose
* xtran(600,600)	real	x transpose
* cccc(600,600)	real	obtained in matmul subroutine
* prod(600,600)	real	obtained in matmul subroutine
* prodin(600,600)	real	obtained in invert subroutine

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

subroutine regres(x,k,n,y,dt,b)

\*DECLARATIONS\*

integer dt,n,k,i,j,regdf,resdf,totdf,pedf,lacdf,nl  
real x(600,600),c(600,600),v(60,60),prodin(600,600),  
+ y(600,600),b(600,600),srot(60),ytran(600,600),prod(600,600),  
k t(60),sum,rsq,freg,flac,SSreg,MSreg,SSregc,SSres,MSres,  
+ SStot,SStotc,SSpe,MSpe,SSlac,MSlac,ccc(600,600),cc(600,600),

```

+ ybar,sumc,ychar,yy,btran(600,600),xtran(600,600),cccc(600,600)

*ALGORITHM*

* calculate degrees of freedom
  totdf=m
  regdf=n
  resdf=m-n

* b=(x'x)inverse*x'y
* SSreg=b'x'y
* SStot=y'y
* SSres=SStot-SSreg
* MSreg=SSreg/regdf
* MStot=SStot/totdf
* MSres=SSres/resdf

  call transp(x,xtran,m,n)

  call matmul(xtran,x,prod,n,m,n)

  call invert(prod,prodin,n)

  call matmul(prodin,xtran,c,n,n,m)

  call matmul(c,y,b,n,m,1)

  call transp(b,btran,n,1)

  call matmul(btran,xtran,cc,1,n,m)

  call matmul(cc,y,ccc,1,m,1)

  SSreg=ccc(1,1)

  call transp(y,ytran,m,1)

  call matmul(ytran,y,cccc,1,m,1)

  SStot=cccc(1,1)

  SSres=SStot-SSreg

  MSreg=SSreg/regdf
  MStot=SStot/totdf
  MSres=SSres/resdf

* calculate the variances of the coefficients
  do 1 i=1,n
    v(i,i)=prodin(i,i)*MSres
  1   continue

* estimated standard errors

```

```

do 22 i=1,n
    srot(i)=sqrt(v(i,i))
22  continue

* calculate t-statistics for each of the coefficients
do 23 i=1,n
    t(i)=b(i,1)/srot(i)
23  continue

* calculate ybar
sum=0.
do 24 i=1,m
    sum=sum+y(i,1)
24  continue
ybar=sum/m

* calculate SSreg corrected for the mean
SSregc=SSreg-(sum*sum)/m

* calculate SStot corrected for the mean
SStotc=SStot-(sum*sum)/m

* calculate residual SS and MS and d.f. due to pure error
if(dt .eq. 1 .or. dt .eq. 2 .or. dt .eq. 3 .or. dt .eq. 5) then
    n1=4
else if (dt .eq. 4 .and. k .eq. 2) then
    n1=8
else if (dt .eq. 4 .and. k .eq. 3) then
    n1=9
else if (dt .eq. 4 .and. k .eq. 4) then
    n1=12
else if (dt .eq. 4 .and. k .eq. 5) then
    n1=10
else if (dt .eq. 4 .and. k .eq. 6) then
    n1=15
else if (dt .eq. 4 .and. k .eq. 7) then
    n1=22
else if (dt .eq. 4 .and. k .eq. 8) then
    n1=20
else if (dt .eq. 4 .and. k .eq. 9) then
    n1=31
else
28  print *, 'Input the # of center points in your design'
    read *, n1
    if (n1 .le. 1) then
        print *, 'You must have more than 1 center point'
        go to 28
    endif
endif
pedf=n1-1

suac=0.
do 25 j=m-n1+1,m

```

```

        sumc=sumc+y(j,1)
25    continue
        ybar=sumc/n1
        yy=0.
        do 26 i=m-n1+1,m
            yy=yy+y(i,1)*y(i,1)
26    continue
        SSpe=yy-(sumc*sumc)/n1
        MSpe=SSpe/pedf

* calculate residual SS and MS and d.f. due to lack of fit
        lacdf=resdf-pedf
        SSLac=SSres-SSpe
        MSLac=SSLac/lacdf

* calculate Rsquare
        rsq=(SSreg/SStotc)

* calculate F test statistic for regression model
        freg=MSreg/MSres

* calculate F test statistic for lack of fit
        flac=MSLac/MSpe

* print regression output *****

        print 100
100    format(11x,'ANOVA for Response Surface Methodology')
        print 200
200    format(11x,'-----')
        print *
        print *
        print *
        print 300
300    format(5x,'SOURCE',9x,'d.f.',9x,'SS',17x,'MS')
        print 400
400    format(5x,'-----')
+ '-----')
        print*
        print 500,'Regression',regdf,SSreg,MSreg
500    format(4x,A14,2x,I2,1x,F18.6,1x,F18.6)
        print 500,'Residual',resdf,SSres,MSres
        print 500,'Pure Error',pedf,SSpe,MSpe
        print 500,'Lack of Fit',lacdf,SSLac,MSLac
        print*
        print 400
        print 600,'Total',totdf,SStot
600    format(4x,A14,2x,I2,1x,F18.6)
        print 400
        print *
        print *
        print *, 'F-statistic for Regression Model= ',freg,'d.f.= ',
+ regdf,',',resdf

```



```

      print *
      print *, 'F-statistic for Lack of Fit= ', flac, ' d.f.= ',
+ lacdf, ',', pedf
      print *
      print *, 'Rsquare (corrected for mean) = ', rsq
      print *
      print *
      print *, '      degrees of freedom for t-statistics= ', m-n
      print *
      print 700
700   format(5x, 'Beta Estimates', 4x, 'standard error(b)', 4x,
+ 't-statistic')
      print 800
800   format(5x, '-----')
      print *
      do 27 i=1,n
          print 900, 'b(', i-1, ')= ', b(i,1), srot(i), t(i)
900   format(5x, A2, I2, A3, F12.5, 1x, F12.5, 5x, F12.5)
27    continue
      print 800

```

\* finished printing regression output \*\*\*\*\*

end

\*\*\*\*\*  
\*\*\*\*\*

\*SUBROUTINE NAME: matmul

\*ARGUMENT LIST: (a,b,c,m,n,p)

\*CALLED BY : regres

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:9 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: multiply matrix A(m\*n) and matrix B(n\*p) and  
\* set equal to C(m\*p)

\*\*\*\*\*

* ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* A(M,N)	IN	REAL	PASSED	MATRIX A
* B(N,P)	IN	REAL	PASSED	MATRIX B
* C(M,P)	OUT	REAL	PASSED	MATRIX C
* M	IN	INTEGER	PASSED	# OF ROWS OF A AND C
* N	IN	INTEGER	PASSED	# OF COL OF A; ROWS OF B
* P	IN	INTEGER	PASSED	# OF COL OF B AND C

\*\*\*\*\*

\*LOCAL VARIABLES:      TYPE:      PURPOSE:

\* i                    integer      used as counter for multiplication  
\* j                    integer      used as counter for multiplication  
\* k                    integer      used as counter for multiplication

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

      SUBROUTINE MATMUL(A,B,C,M,N,P)

\*DECLARATIONS\*

      INTEGER N,M,P,I,J,K  
      REAL A(600,600),B(600,600),C(600,600),SUM

\*ALGORITHM\*

      DO 20 I = 1,M  
        DO 10 J = 1,P  
          SUM = 0.0  
          DO 5 K = 1,N  
            SUM = SUM + A(I,K) \* B(K,J)  
5          CONTINUE  
          C(I,J) = SUM  
10        CONTINUE  
20        CONTINUE

      END

\*\*\*\*\*  
\*\*\*\*\*  
\*SUBROUTINE NAME: transp

\*ARGUMENT LIST: (a,b,m,n)  
\*CALLED BY     : regres

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:9 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: takes a matrix A (m\*n) and computes its  
\*                    transpose matrix B (n\*m)

\*\*\*\*\*

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
# NAME	OUT		GLOBAL	
* A(600,600)	IN	REAL	PASSED	MATRIX A
* B(600,600)	OUT	REAL	PASSED	MATRIX B
* M	IN	INTEGER	PASSED	# ROWS OF A
* N	IN	INTEGER	PASSED	# COLUMNS OF A

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	# rows of A
* j	integer	# columns of A

\*\*\*\*\*  
\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

SUBROUTINE TRANSP(A,B,M,N)

\*DECLARATIONS\*

INTEGER M,N,I,J  
REAL A(600,600),B(600,600)

\*ALGORITHM\*

```

DO 20 I = 1,M
  DO 10 J = 1,N
    B(J,I) = A(I,J)
10  CONTINUE
20  CONTINUE

END

```

\*\*\*\*\*  
\*\*\*\*\*

\*SUBROUTINE NAME: uncode

\*ARGUMENT LIST: (b,min,max,dt,k,order)  
\*CALLED BY : main

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:12 October

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

\*\*\*\*\*

\*MODULE DESCRIPTION: This subroutine uncodes the beta estimates  
\* obtained in the regression subroutine

\*\*\*\*\*

*ARGUMENTS:	IN/	TYPE	PASSED/	PURPOSE
* NAME	OUT		GLOBAL	
* b(600,600)	in	real	passed	beta estimates from reg
* min(10)	in	real	passed	minimum levels of factors
* max(10)	in	real	passed	maximum levels of factors
* dt	in	integer	passed	design type
* k	in	integer	passed	# of factors
* order	in	integer	passed	design order if dt=6

\*\*\*\*\*

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* ii	integer	used as a counter
* jj	integer	used as a counter
* i	integer	used as a counter
* il	integer	used as a counter
* cj	integer	used as a counter
* nn	integer	used as a counter
* den(10)	real	range(10)/2.
* range(10)	real	range of factors
* ave(10)	real	average of factors
* nb(600,600)	real	new uncoded betas
* add	real	add to nb(0)
* add0	real	add to nb(0)
* add1(11)	real	add to nb linear
* add00	real	add to nb(0)
* add11(11)	real	add to nb linear
* add12(11)	real	add to nb linear
* add000	real	add to nb(0)

\*\*\*\*\*

\*\*\*\*\*

\*BEGINNING OF ACTUAL FORTRAN CODE\*

subroutine uncode(b,min,max,dt,k,order)

\*DECLARATIONS\*

integer dt,k,order,ii,jj,i,il,cj,nn  
real b(600,600),min(10),max(10),den(10),range(10),ave(10),  
+ nb(600,600),add,add0,add1(11),add00,add11(11),add12(11),add000

\* find out if design type is first order or second order if user dt

if (dt .eq. 6 .and. order .eq. 1) then

dt=61

endif

if (dt .eq. 6 .and. order .eq. 2) then

dt=62

endif

\* calculate ranges and averages for each of the factors

```

* also calculate denominators to be used in calculations
do 1 i=1,k
    range(i)=max(i)-min(i)
    ave(i)=(max(i)+min(i))/2.
    den(i)=range(i)/2.
1    continue

* calculate uncoded beta estimates if design type is first order
if (dt .eq. 1 .or. dt .eq. 2 .or. dt .eq. 61) then
    add=0.
    do 2 i=2,k+1
        ii=i-1
        nb(i,1)=b(i,1)/den(ii)
        add=add+(-(b(i,1)*ave(ii))/den(ii))
2    continue
    nb(1,1)=b(1,1)+add
    print *
    print *
    print 100
100   format(5x,'Uncoded Beta Estimates')
    print 200
200   format(5x,'-----')
    print *
* print uncoded coefficients
    do 3 i=1,k+1
        print 300,'b(',i-1,')= ',nb(i,1)
300   format(5x,A2,I2,A3,F12.5)
3    continue
    print 200
endif

* calculate uncoded beta estimates if design type is second order
if (dt .eq. 3 .or. dt .eq. 4 .or. dt .eq. 5 .or. dt .eq. 62) then

* calculate initial uncoded linear coefficients and change b(0)
    add0=0.
    do 4 i=2,k+1
        ii=i-1
        nb(i,1)=b(i,1)/den(ii)
        add0=add0+(-(b(i,1)*ave(ii))/den(ii))
4    continue

* calculate squared coefficients, change linear and change b(0)
    do 5 i=2,11
        add1(i)=0.
5    continue
    add00=0.
    do 6 i=k+2,2*k+1
        ii=i-(k+1)
        nb(i,1)=b(i,1)/(den(ii)*den(ii))
        add1(i-k)=add1(i-k)+(-(2*b(i,1)*ave(ii))/
+          (den(ii)*den(ii)))
        add00=add00+(b(i,1)*(ave(ii)*ave(ii))/(den(ii)*den(ii)))

```

```

6      continue

* calculate interaction coefficients, change linear and change b(0)
      add000=0.
      do 7 i=2,11
          add11(i)=0.
          add12(i)=0.
7      continue
      cj=2
      nn=2*k+2
      do 8 ii=1,k-1
          do 9 jj=cj,k
              nb(nn,1)=b(nn,1)/(den(ii)*den(jj))
              add11(ii+1)=add11(ii+1)+(-(b(nn,1)*ave(jj)))/
              +
              (den(jj)*den(ii))
              add12(jj+1)=add12(jj+1)+(-(b(nn,1)*ave(ii)))/
              +
              (den(ii)*den(jj))
              add000=add000+(b(nn,1)*ave(jj)*ave(ii))/
              +
              (den(jj)*den(ii))
              nn=nn+1
9      continue
      cj=cj+1
8      continue

* print uncoded coefficients
      print *
      print *
      print 400
400     format(5x,'Uncoded Beta Estimates')
      print 500
500     format(5x,'_____')
      print *
* beta(0) coefficient
      print *, '    b(0)=    ',b(1,1)+add0+add00+add000

* linear coefficients
      do 11 i=2,k+1
          print 700,'b(',i-1,')=    ',nb(i,1)+add1(i)+add11(i)
          +
          +add12(i)
700     format(5x,A2,I1,A5,F12.7)
11      continue

* squared coefficients
      il=1
      do 12 i=k+2,2*k+1
          print 800,'b(',i1,',',i1,')=    ',nb(i,1)
800     format(5x,A2,I1,A1,I1,A3,F12.7)
          il=il+1
12      continue

* interaction coefficients
      cj=2
      nn=2*k+2

```

```

do 13 ii=1,k-1
do 14 jj=cj,k
print 900,'b(',ii,',',jj,')= ',nb(nn,1)
900    format(5x,A2,I1,A1,I1,A3,F12.7)
nn=nn+1
14    continue
cj=cj+1
13    continue
print 500

```

endif

end

```

*****
*****
*SUBROUTINE NAME: copy

```

```

*ARGUMENT LIST: (a,b,m,n)
*CALLED BY      : main

```

\*CLASS: sm799 PROJECT: Thesis Research ADVISOR: Cook DATE:29 Sept

\*NAME OF PROGRAMMER: Kalla Sparrow (LOGIN NAME: ksparrow)

```

*****

```

\*MODULE DESCRIPTION: copies matix a to matrix b

```

*****

```

*ARGUMENTS:	IN/ OUT	TYPE	PASSED/ GLOBAL	PURPOSE
* NAME				
* a(600,600)	in	real	passed	generated design matrix
* b(600,600)	out	real	passed	copied design matrix
* m	in	integer	passed	# of rows of a and b
* n	in	integer	passed	# of columns of a and b

```

*****

```

*LOCAL VARIABLES:	TYPE:	PURPOSE:
* i	integer	used for row counter
* j	integer	used for column counter

```

*****
*****

```

```

*BEGINNING OF ACTUAL FORTRAN CODE*
subroutine copy(a,b,m,n)

```

```

*DECLARATIONS*
integer m,n,i,j
real a(600,600),b(600,600)

```

```

      do 1 i=1,m
        do 2 j=1,n
          b(i,j)=a(i,j)
2       continue
1       continue

      end

```

```

*****
*****

```

```

      SUBROUTINE INVERT(X,XX,N)
*      FORTRAN PROGRAM FOR CALCULATING THE INVERSE OF A
*      GIVEN MATRIX
*
*      REFERENCE IS CONTE, S.D. AND CARL DE BOOR,ELEMENTARY NUMERICAL
*      ANALYSIS: AN ALGORITHMIC APPROACH, MCGRAW-HILL BOOK COMPANY,
*      3RD EDITION, 1980.

```

```

      DIMENSION A(360000),AINV(360000),B(600),IPIVOT(600),
+ X(600,600),XX(600,600)
      NSB =N*N
      DO 10 I=1,N
      DO 10 J=1,N
10     A((I-1)*N+J)=X(I,J)
*

```

```

      CALL FACTOR(A,A,IPIVOT,B,N,IFLAG)
      GO TO (20,11),IFLAG
11     PRINT 611
611    FORMAT(' ','MATRIX IS SINGULAR')
      GO TO 1
20     DO 21 I=1,N
21     B(I)=0.
      IBEG=1
      DO 30 J=1,N
      B(J)=1.
      CALL SUBST(A,B,AINV(IBEG),IPIVOT,N)
      B(J) = 0.
30     IBEG = IBEG+N
      DO 15 I=1,N
      K=1
      DO 16 J=1,NSB,N
      XX(I,K)=AINV(J)
      K=K+1
16     CONTINUE
15     CONTINUE
      GO TO 1
1     END
*
*

```

```

      SUBROUTINE FACTOR(A,W,IPIVOT,D,N,IFLAG)
      DIMENSION A(N,N),W(N,N),IPIVOT(N),D(N)
      IFLAG =1

```



```

*      INITIALIZE W, IPIVOT,D
      DO 10 I=1,N
      IPIVOT(I)=I
      ROWMAX=0.
      DO 9 J=1,N
9      ROWMAX=AMAX1(ROWMAX,ABS(W(I,J)))
      IF (ROWMAX.EQ.0.) GO TO 999
10     D(I)=ROWMAX
*      GAUSS ELIMINATION WITH SCALED PARTIAL PIVOTING
      NM1=N-1
      IF(NM1.EQ.0) RETURN
      DO 20 K=1,NM1
      J=K
      KP1=K+1
      IP=IPIVOT(K)
      COLMAX=ABS(W(IP,K))/D(IP)
      DO 11 I=KP1,N
      IP=IPIVOT(I)
      AMIKOV=ABS(W(IP,K))/D(IP)
      IF(AMIKOV.LE.COLMAX) GO TO 11
      COLMAX=AMIKOV
      J=I
11     CONTINUE
      IF(COLMAX.EQ.0.) GO TO 999
*
      IPK=IPIVOT(J)
      IPIVOT(J)=IPIVOT(K)
      IPIVOT(K)=IPK
      DO 20 I=KP1,N
      IP=IPIVOT(I)
      W(IP,K)=W(IP,K)/W(IPK,K)
      RATIO=-W(IP,K)
      DO 20 J=KP1,N
20     W(IP,J)=RATIO*W(IPK,J)+W(IP,J)
      IF(W(IP,N).EQ.0.) GO TO 999
      RETURN
999    IFLAG=2
      RETURN
      END
**
**
      SUBROUTINE SUBST(W,B,X,IPIVOT,N)
      DIMENSION W(N,N),B(N),X(N),IPIVOT(N)
      IF(N.GT.1) GO TO 10
      X(1)=B(1)/W(1,1)
      RETURN
10     IP=IPIVOT(1)
      X(1)=B(IP)
      DO 15 K=2,N
      IP=IPIVOT(K)
      KM1=K-1
      SUM=0.
      DO 14 J=1,KM1

```

```

14      SUM=W(IP,J)*X(J)+SUM
15      X(K)=B(IP)-SUM
        X(N)=X(N)/W(IP,N)
        K=N
        DO 20 NP1MK=2,N
        KP1=K
        K=K-1
        IP=IPIVOT(K)
        SUM=0.
        DO 19 J=KP1,N
19      SUM=W(IP,J)*X(J)+SUM
20      X(K)=(X(K)-SUM)/W(IP,K)
        RETURN
        END

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## Appendix C. Design Listings

### 2 Factor Full 2<sup>k</sup> Design

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3 Factor Full 2\*\*k Design

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7 Factor Full 2<sup>++</sup>k Design

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AD-A151 956

AN INTERACTIVE COMPUTER PACKAGE FOR USE WITH SIMULATION 3/5

MODELS WHICH PERF. (U) AIR FORCE INST OF TECH

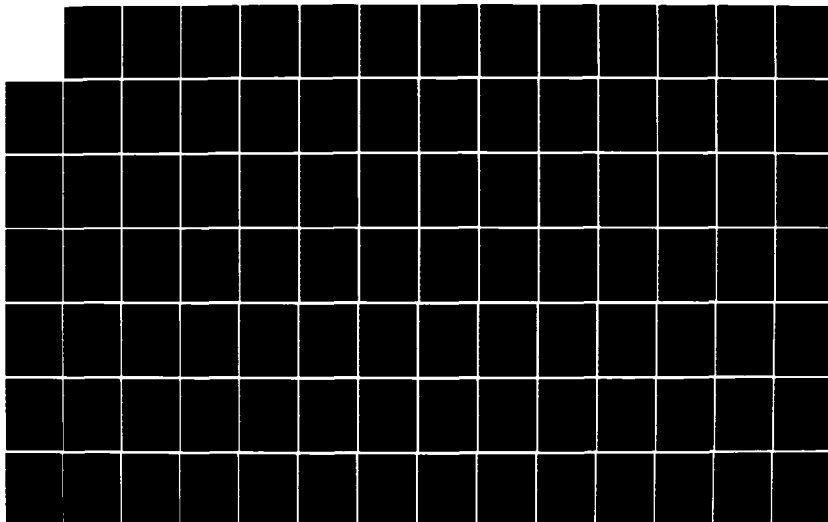
WRIGHT-PATTERSON AFB OH SCHOOL OF ENGI... K J SPARROW

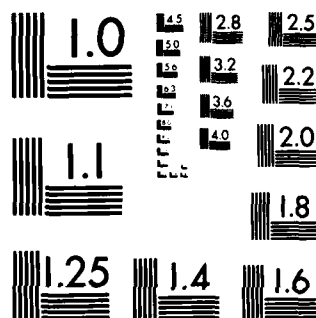
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MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS-1963 A

8 Factor Full 2<sup>16</sup>k Design

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2 Factor Fractional 2<sup>4</sup>k Design

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### 3 Factor Fractional 2<sup>4</sup>-k Design

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4 Factor Fractional 2<sup>5</sup>k Design (25:308)

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1.000 1.000 1.000 1.000 1.000

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5 Factor Fractional 2<sup>4</sup>k Design (16:277)

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1.000-1.000-1.000 1.000 1.000-1.000

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6 Factor Fractional 2<sup>16</sup>-k Design (16:278)

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1.000-1.000 1.000-1.000 1.000-1.000 1.000

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7 Factor Fractional 2<sup>8</sup>k Design (16:280)

1.000-1.000-1.000-1.000-1.000-1.000-1.000-1.000
1.000-1.000 1.000-1.000 1.000-1.000 1.000 1.000
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B Factor Fractional 2\*\*k Design (22:41)

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1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
1.000	1.000	-1.000	1.000	-1.000	1.000	-1.000	-1.000	1.000
1.000	-1.000	1.000	-1.000	1.000	-1.000	1.000	1.000	-1.000
1.000	1.000	1.000	-1.000	-1.000	1.000	1.000	-1.000	-1.000
1.000	1.000	-1.000	-1.000	1.000	1.000	-1.000	1.000	-1.000
1.000	1.000	1.000	1.000	1.000	-1.000	-1.000	-1.000	-1.000
1.000	-1.000	-1.000	-1.000	-1.000	1.000	1.000	1.000	1.000
1.000	-1.000	1.000	-1.000	1.000	1.000	-1.000	-1.000	1.000
1.000	1.000	-1.000	1.000	-1.000	-1.000	1.000	1.000	-1.000
1.000	1.000	1.000	-1.000	-1.000	-1.000	-1.000	1.000	1.000
1.000	-1.000	-1.000	1.000	1.000	1.000	1.000	-1.000	-1.000
1.000	-1.000	1.000	1.000	-1.000	1.000	-1.000	1.000	-1.000
1.000	1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	1.000
1.000	-1.000	1.000	1.000	-1.000	1.000	-1.000	-1.000	1.000
1.000	-1.000	-1.000	1.000	1.000	-1.000	1.000	1.000	-1.000
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9 Factor Fractional 2<sup>k</sup> Design (22; 42)

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#### 6 Factor Full $3^k$ Design

You input  $k = 6$

For  $k > 5$  the full  $3^k$  design requires too many runs.

Change your input design type to either 4 or 5.

The CCD and Fractional  $3^k-p$  are more efficient.

To change this limitation recode subroutine full3k.

## 2 Factor Central Composite Design

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### 3 Factor Central Composite Design

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#### 4 Factor Central Composite Design

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5 Factor Central Composite Design (22:5)

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7 Factor Central Composite Design (22:7)

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8 Factor Central Composite Design (22:20)

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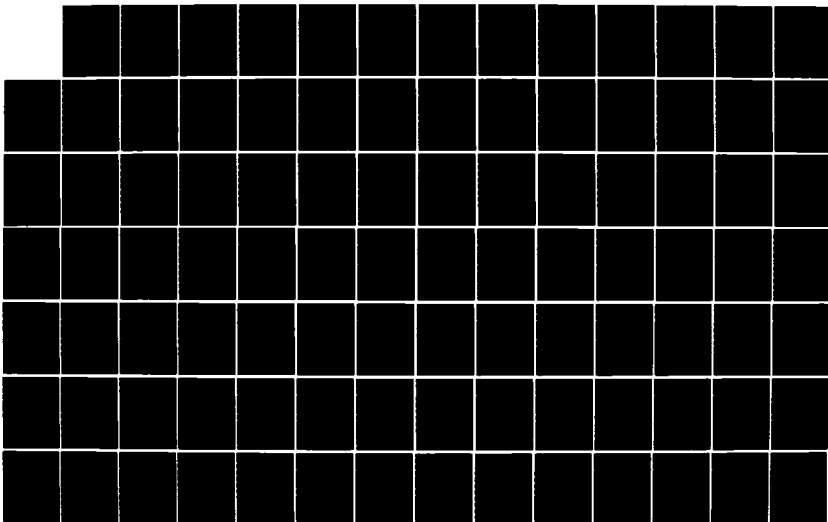
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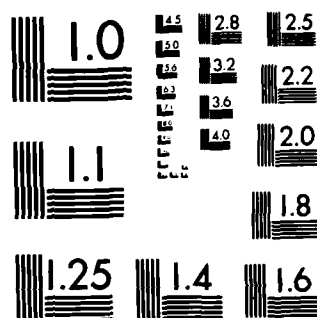




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MICROCOPY RESOLUTION TEST CHART  
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#### 4 Factor Fractional 3<sup>4</sup>k Design

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# 5 Factor Fractional 3<sup>5</sup>k Design (17:11)

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6 Factor Fractional 3<sup>2</sup>k Design (17:13)

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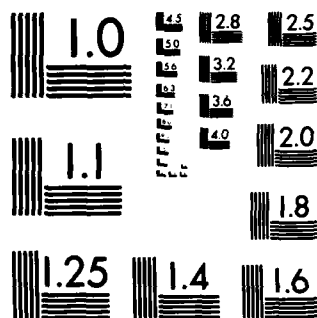
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**C-217**

9 Factor Fractional 3\*\*k Design (17:31-32)

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